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VOL III

EVALUATION AND PREDICTION OF HENRY'S LAW CONSTANTS AND AQUEOUS SOLUBILITIES FOR SOLVENTS AND HYDROCARBON FUEL COMPONENTS
VOL III: EXPERIMENTAL SOLUBILITY DATA

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Volatile organics, solvents, fuels, Henry's law constants, aqueous solubilities, air-water distribution.

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Laboratory measurements of Henry's law constants are reported for 51 chemicals spanning a wide range of chemical structures and volatilities. A static headspace method (Equilibrium Partitioning in Closed Systems, referred to as EPICS) was used to measure Henry's Law Constant, with the standard batch air-stripping method used as a check. An average precision of 5 percent was obtained for the EPICS runs, and the Henry's law constants agreed reasonably well (within 10 percent) with the batch air-stripping results and other reported experimental values. Measurements were conducted over a temperature range of 10-30°C, and the data were correlated with a temperature regression equation coupled with a temperature-dependent error term based on 95 percent confidence limits. The aqueous solubilities of the study compounds were also determined via the shake-flask method at temperatures of 10, 20, and 30 degrees Celsius. Finally, the results of this study were incorporated into a thermodynamic correlation (UNIFAC), based on chemical structure, which allows the prediction of Henry's law constants and aqueous solubilities for a wide variety of pure compounds and mixtures (Cont'd)

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ITEM 19. ABSTRACT (Cont'd)

in dilute aqueous solutions. Volume III: Experimental Solubility Data (Volume III of III)

This report is presented in three volumes. Volume I contains the technical discussion and fabulated values of Henry's law constants and aqueous solubilities. Volume II contains the experimental Henry's law data. Volume III contains the experimental solubility data and the Fortran source code for the simplex UNIFAC parameter fitting and the interactive program for calculating Henry's law constants and aqueous solubilities.

EXECUTIVE SUMMARY

The Installation Restoration program (IRP) underway at numerous Air Force bases has identified several sites with contaminated soil and groundwater. This subsurface contamination is the result of fuels, cleaning solvents, and degreasers entering the subsurface environment from accidental spills, leaking storage tanks, and past disposal practices. HQ AFESC/RDVW is conducting research aimed at developing treatment strategies for groundwater cleanup, and studying the fate and transport of contaminants in subsurface systems. Many of the contaminants of concern are volatile by nature, and a knowledge of their air-water distribution and aqueous solubility is needed to assess the compounds treatability and to support the basic laboratory studies.

The objectives of this research were to develop Henry's law constants and aqueous solubilities as a function of temperature, for a variety of organic compounds of Air Force concern ~~(Table 1)~~. Secondary objectives were to determine what effect mixed organics, in an aqueous solution, exhibit on individual Henry's law constants and evaluate various methods used to predict Henry's law constants.

This report documents experimentally determined values of Henry's law constants and aqueous solubility for 51 compounds of Air Force concern. The report is presented in three volumes. Volume I contains the technical discussion and tabulated values of Henry's law constants and aqueous solubilities. Volume II and III contain all the raw data and the fortran source code for an interactive program used to predict the chemical parameters.

Many of the contaminants of concern are volatile by nature, and a knowledge of their air-water distribution is required for the design of treatment processes and for providing insight into their environmental fate and transport. A static headspace method (Equilibrium Partitioning In Closed Systems, referred to as EPICS) was used to measure the Henry's law constants, with the standard batch air stripping method used as a check.

The Henry's constants were determined as a function of tempertaure from 10 to 30 ^{o}C (Table 11) and these values were then used to generate temperature regression equations (Table 8). Generally speaking the EPICS' results from this study agree well with other published results (Table 12). However, for many of the compounds reported here, confirmed values of Henry's constant do not exist in the literature, and if they do, values are rarely reported as a function of temperature with rigorous statistics.

Solubility data for organic compounds in water are important for environmental studies because they provide fundamental information necessary to predict transport in aqueous systems. This data may also be used to predict carbon sorption of contaminants, and the air- or stream-stripping behavior for a given compound. The aqueous solubility of the 51 study

compounds were determined at 10, 20, and 30°C (Table 14). Three different methods were used, but the majority of the data were collected using a shake-flask technique. Although the solubilities were not a strong function of temperature over the range studied (i.e., 10-30 °C), several general trends were noted. First, the solubility of the halongenated hydrocarbons increased with temperature. Second, the solubility of the substituted aromatic hydrocarbons increased with temperature. Finally, maxima and minima are observed for a wide range of compounds without any general trend that can be demonstrated to be statistically significant.

Groundwater contamination is often characterized by the presence of several different contaminants rather than one single compound. For this reason, studies were conducted to determine whether the presence of other compounds would affect the Henry's law constant of a single compound. Deviations from ideal behavior were observed (pg 52), but confirming experiments were not performed. Although the results were not conclusive, the project team believes the observed interactions were real and reproducible.

It would not be feasible to experimentally determine Henry's law constants for all chemical compounds. There will be times when a Henry's law constant is needed but an experimentally determined value is not reported and the situation does not permit a laboratory study to determine the constant. For this reason, a technique to accurately estimate Henry's constant using a minimum of physiochemical properties would be useful. Three different thermodynamic techniques for correlating experimental Henry's law constants were examined (page 61). The techniques were examined to determine their applicability to environmental systems and their predictive capacity for unmeasured multicomponent systems. The UNIFAC method proved to be the most effective way of utilizing the data base developed during this project. A computer algorithim to fit the current data to a new environmental UNIFAC binary interaction data base was developed and a portion of the experimental data collected was incorporated into this new data base. The new data base creates improvement in the predictions generated by UNIFAC in the dilute concentration regime (Figures 13 through 16).

PREFACE

This report was prepared by the Research Triangle Institute, Research Triangle Park NC 22707, under Contract No. F08635-85-C-0054. The AFESC/RDVW Project Officer was Captain Richard A. Ashworth.

The report documents Henry's law constants and aqueous solubilities, as a function of temperature, for 51 compounds of Air Force concern. The study was performed between February 1985 and September 1986.

This report is presented in three volumes. Volume I contains the technical discussion and the tabulated values of Henry's law constants and aqueous solubilities. Volume II contains the experimental Henry's law data. Volume III contains the experimental solubility data and the Fortran source code for the simplex UNIFAC parameter fitting and the interactive program for calculating Henry's law constants and aqueous solubilities.

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This report has been reviewed by the Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

Richard A. Ashworth

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Project Officer

LAWRENCE D. HOKANSON, Lt Col, USAF
Director, Engineering and Services Laboratory

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Chief, Environics Division

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APPENDIX C

SUMMARY OF AQUEOUS SOLUBILITY MEASUREMENTS

This is a self-contained document with its own internal style, which varies from our format.

SOLUBILITY MEASUREMENTS

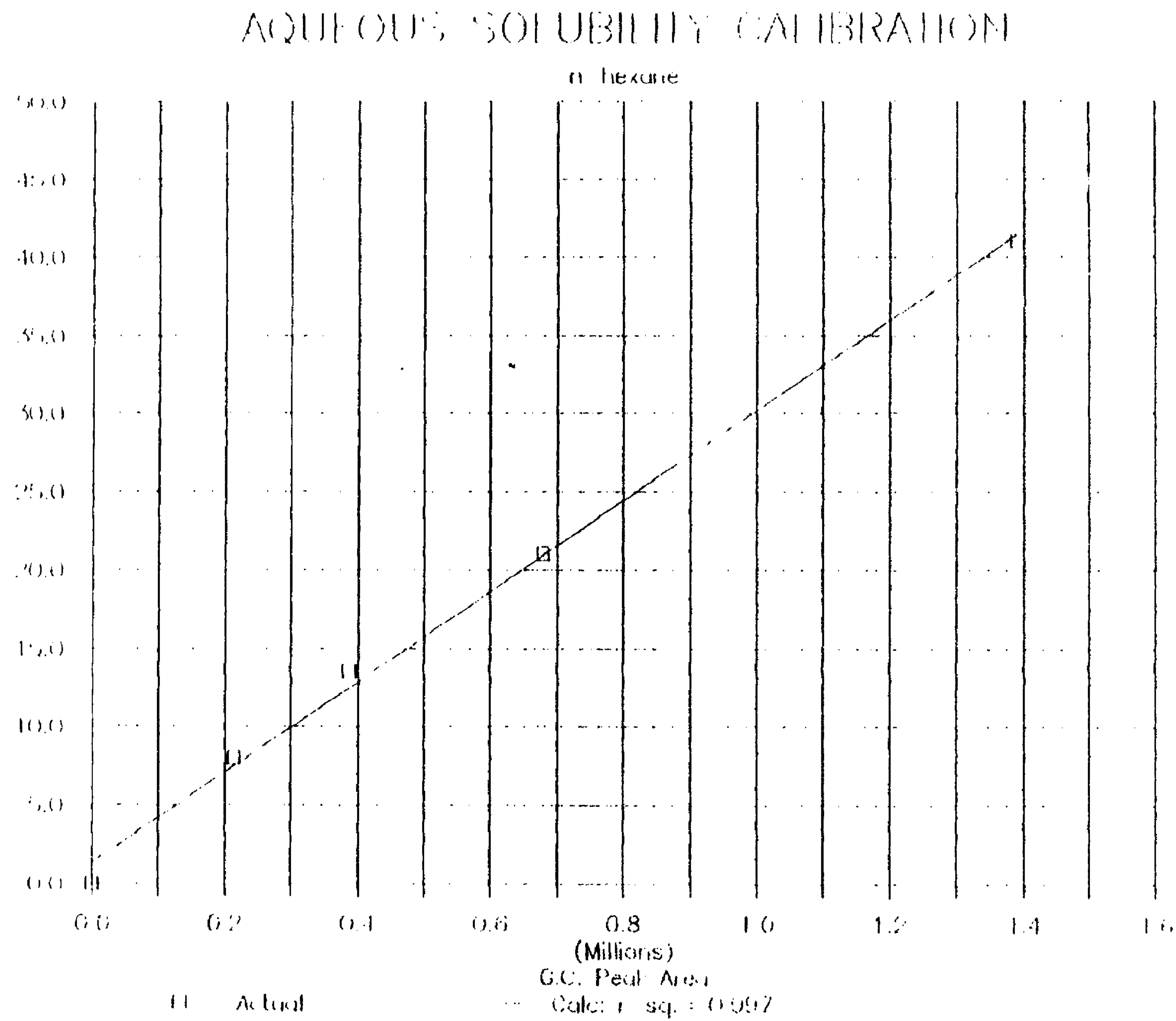
The shake-flask measurements to determine solubility required several calibration points to insure their statistical validity. In this study, at least five independently prepared solutions of unknown concentration were calibrated against the response of the measurement instrument. (In many, if not most, previous studies serial dilutions of one sample were used instead). In the case of aromatic compounds this instrument was a ultra violet (U.V.) spectrometer. The calibration samples were prepared with distilled water in gas tight amber bottles containing no headspace. Since water was employed for U.V. tests, only concentration below the saturation level could be prepared. In some cases, these calibration samples might be too far below the measured U.V. response and additional samples closer to the true solubility limit would be prepared.

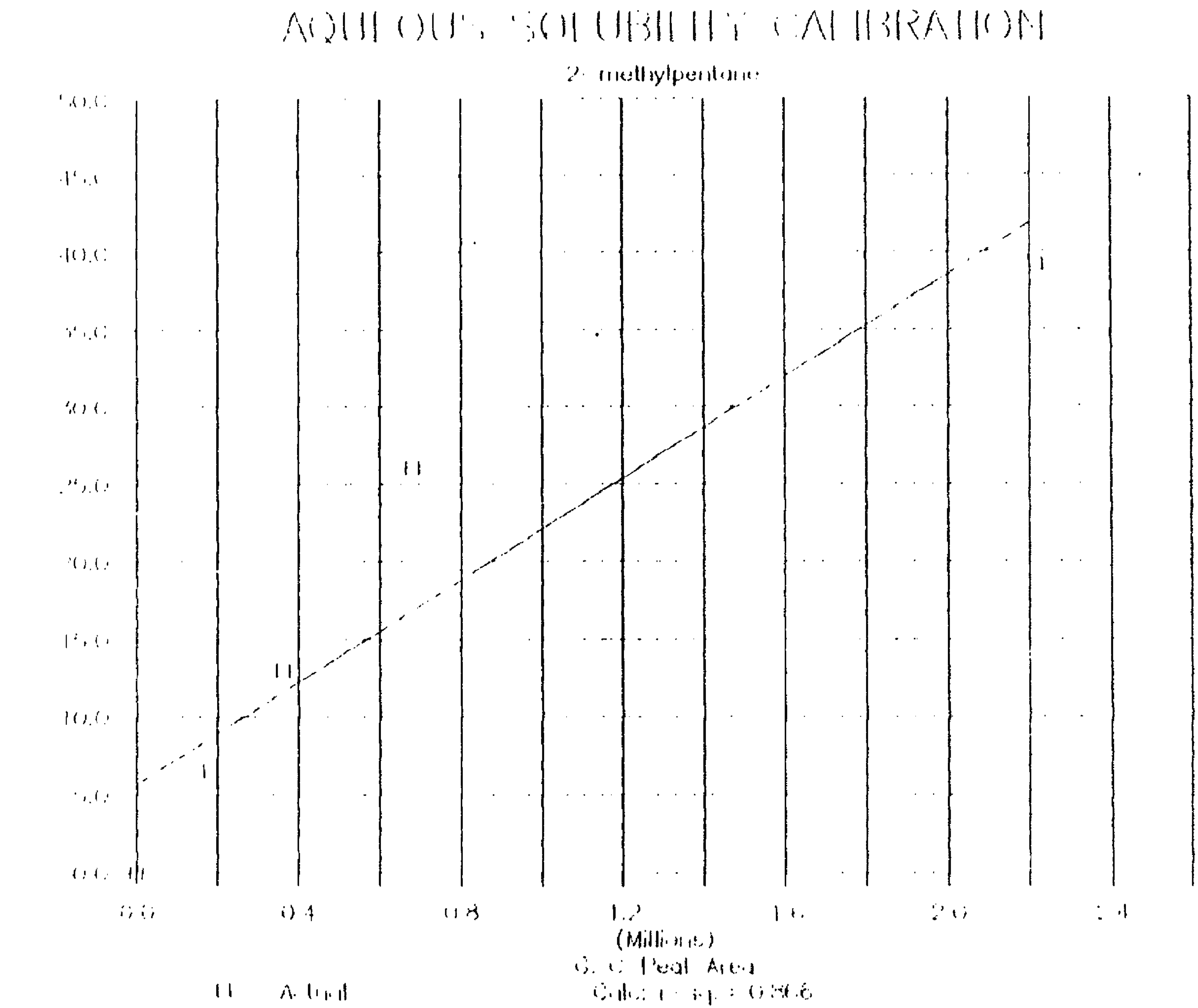
The data was logged onto a Lotus(R) spreadsheet and a linear regression of the calibration concentrations versus detector response determined. The detector response for the saturated solution at all three temperatures could then be entered, and the corresponding solubility limits determined from extrapolation of the linear regression.

In the case of the gas chromatograph samples, a similar scheme was employed using integrator peak area as the detector response instead of U.V. absorbance. In this case, however, calibration samples were prepared in methanol, so calibration concentrations above the aqueous solubility limit might be prepared.

Based upon the correlation coefficient for the linear regression fit on the calibration samples (which is shown in the following plots), 95 percent confidence bands can be placed on the saturated simple concentrations. These are also shown on the following plots. Notice, of course, that the better the correlation coefficient the narrower the bands. Unfortunately, in most cases (even with correlation coefficients in excess of 0.95), little statistical confidence may be placed in the temperature dependency of the solubilities measures. As a consequence, the data has not been tabulated explicitly as a function of temperature dependence.

The nephelometry results are not listed in the same fashion as the other results due to differences in the preparation procedure. However, a discussion of the statistics of nephelometry is contained in Section IV of the main text.


AQUEOUS SOLUBILITY CALIBRATION
n hexane
50.0
45.0
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
(Millions)
G.C. Peak Area
Actual
Calc: r sq. = 0.997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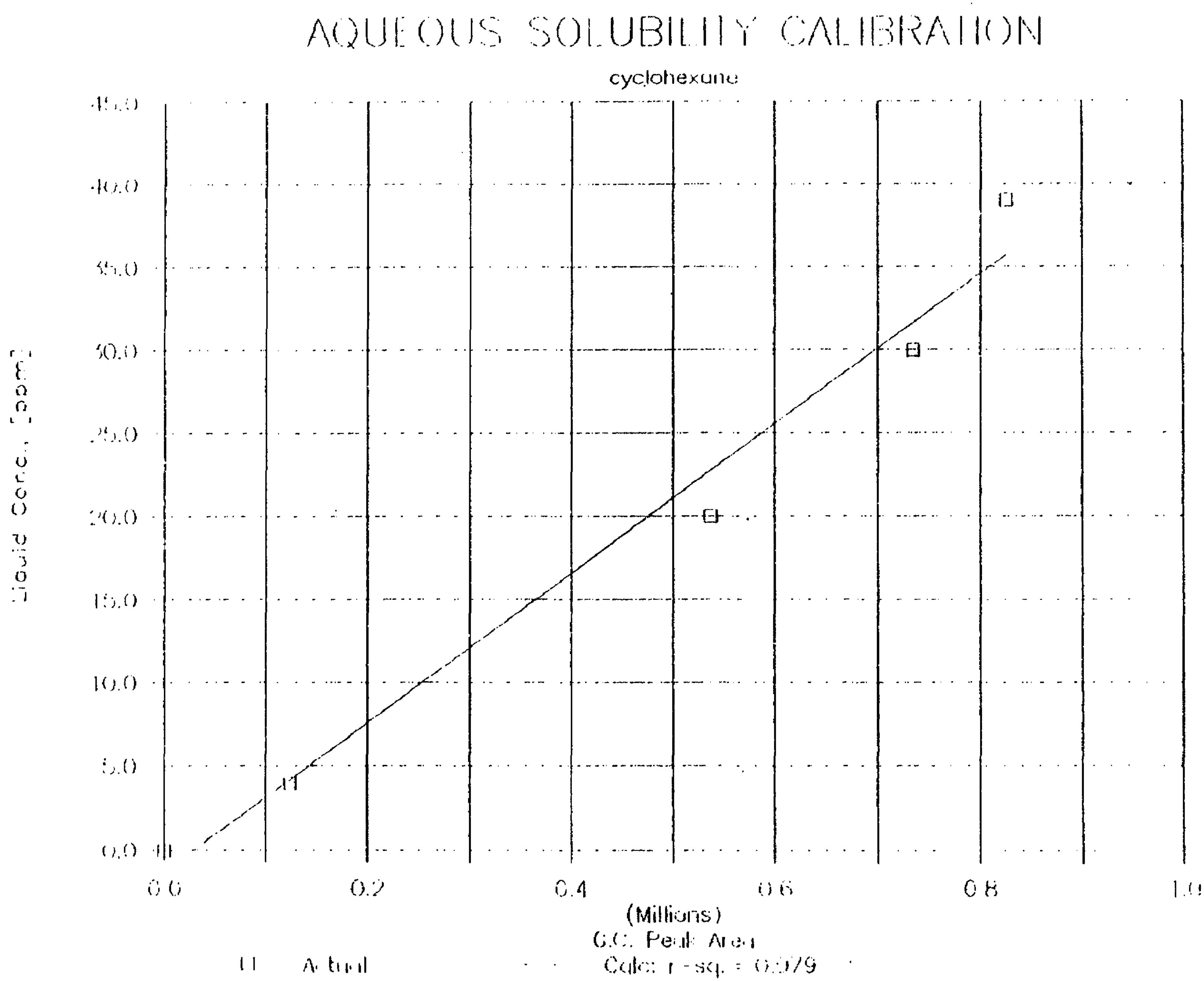
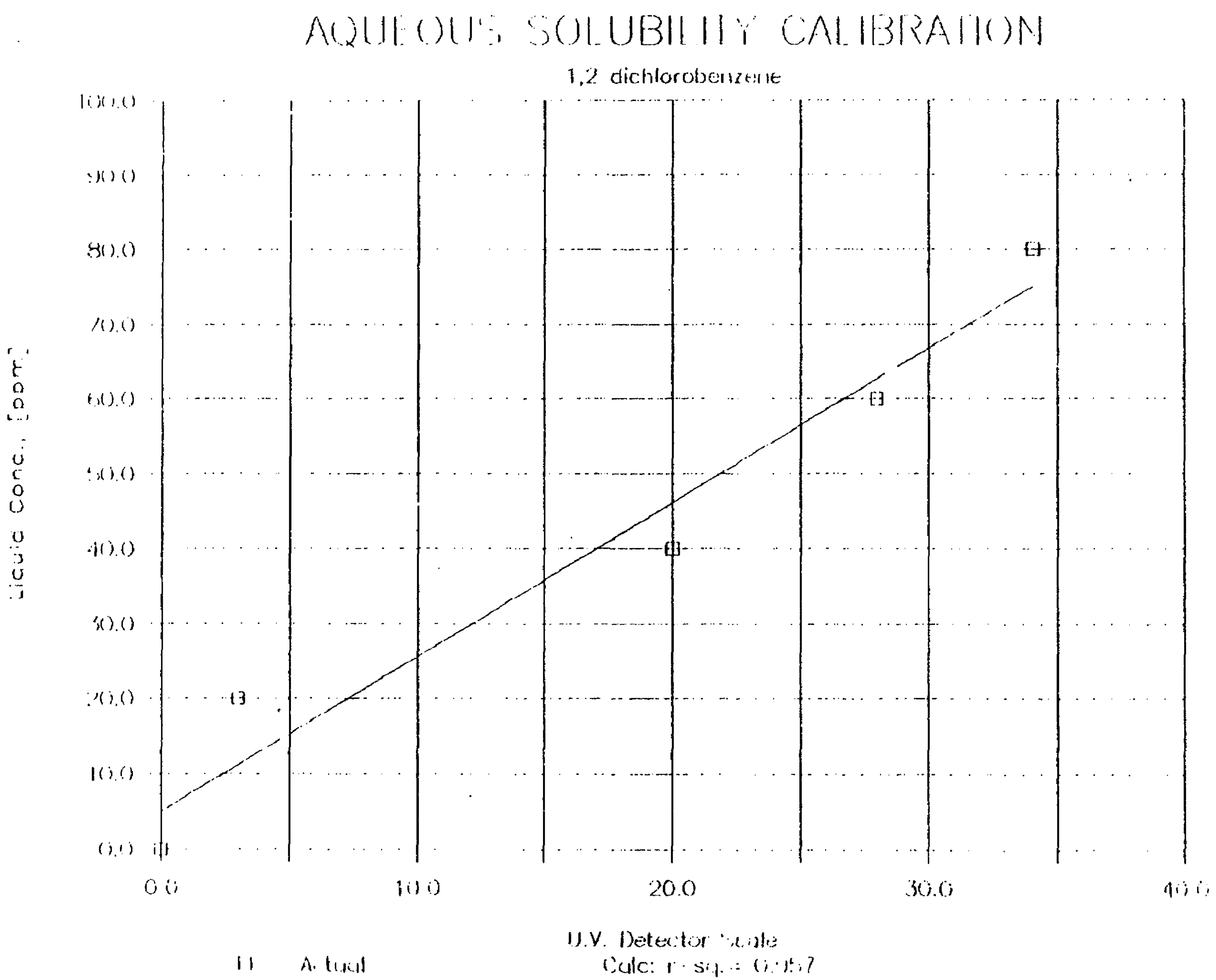
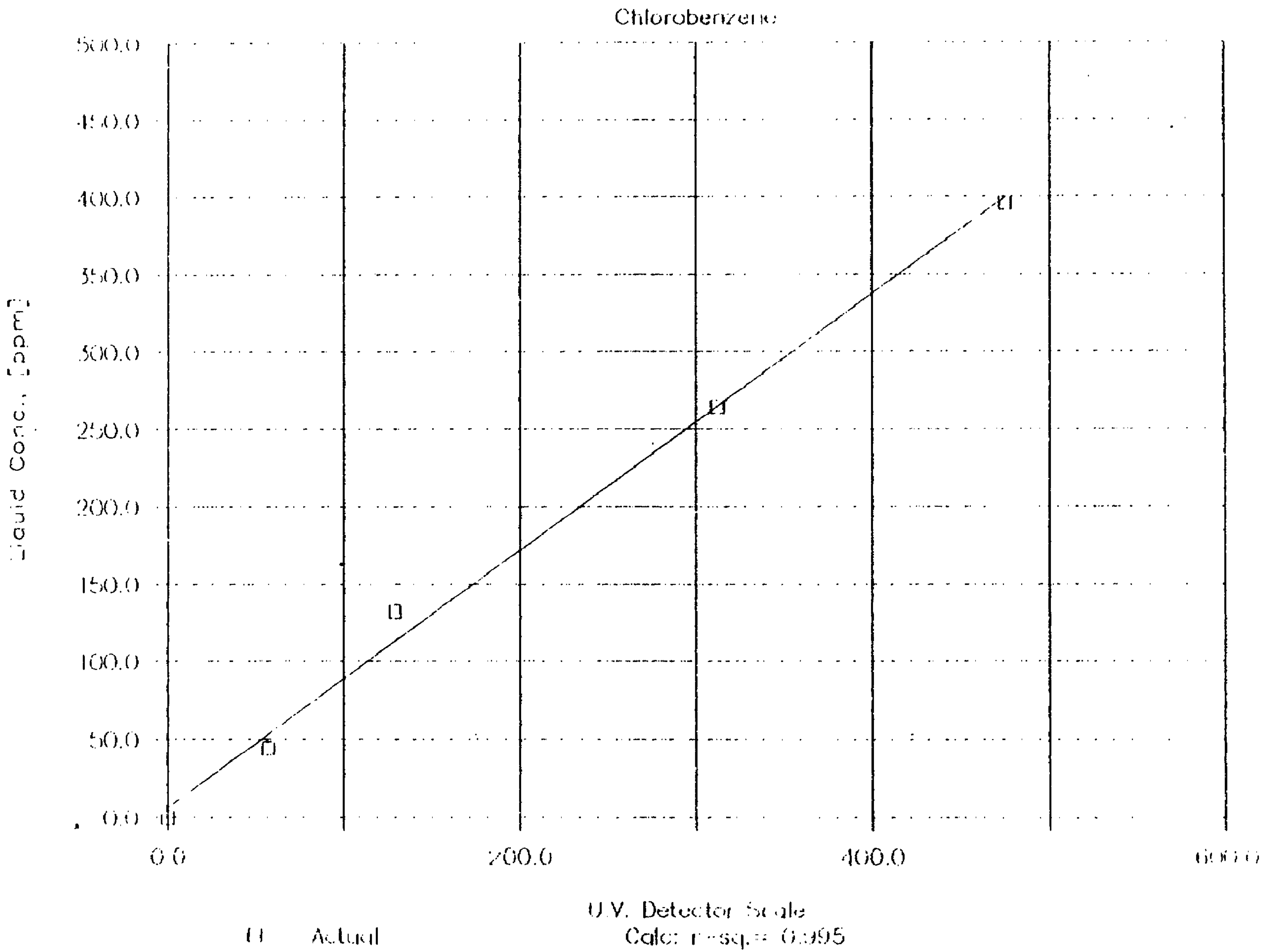
2- methylpentane
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0
0.0
0.4
0.8
1.2
1.6
2.0
2.4
(Millions)
G. C. Peak Area
Actual


AQUEOUS SOLUBILITY CALIBRATION
cyclohexane
Liquid Conc., [ppm]
45.0
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
0.0
0.2
0.4
0.6
0.8
1.0
(Millions)
G.C. Peak Area
Actual
Calc: r-sq. = 0.979

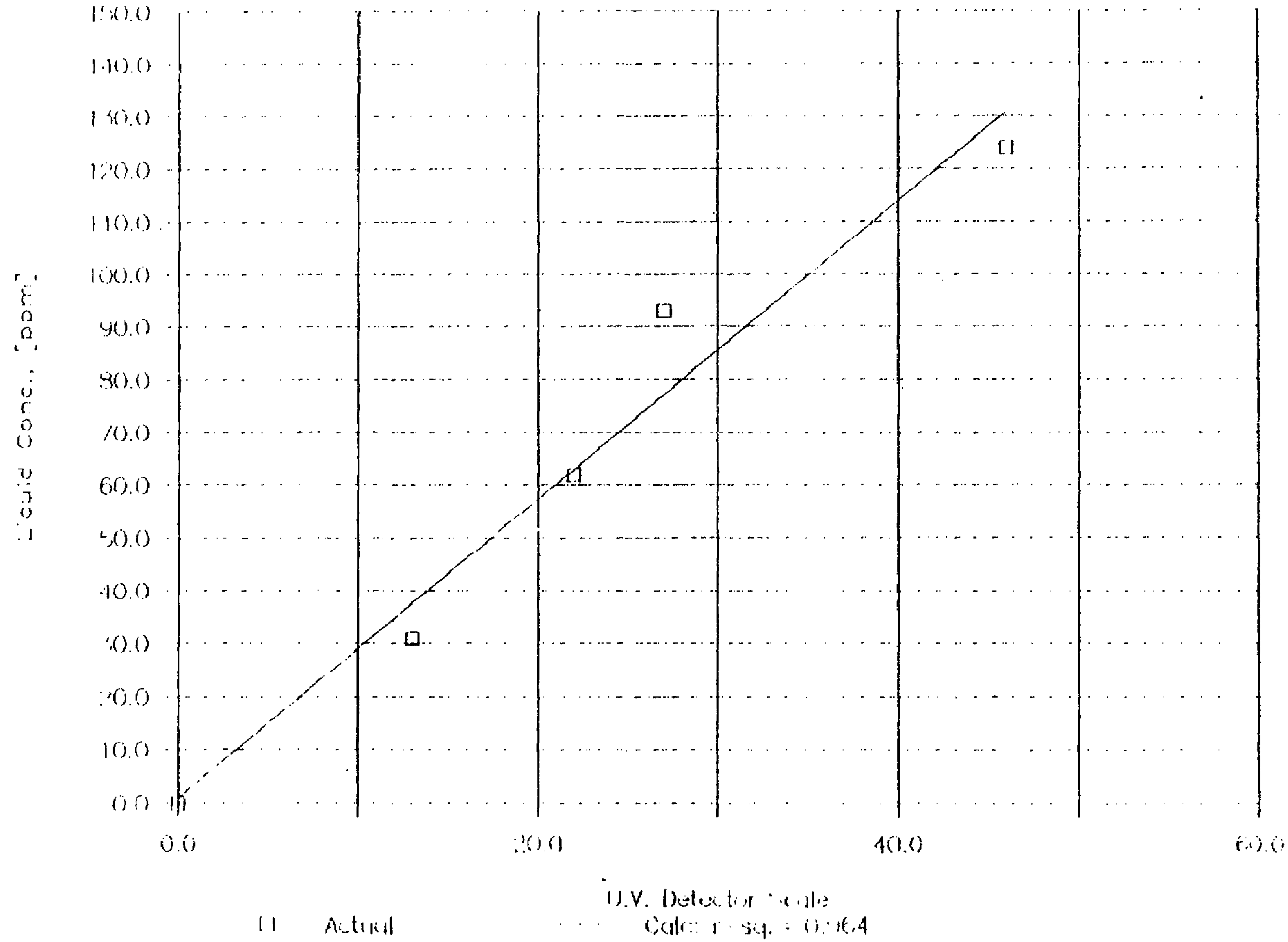

AQUEOUS SOLUBILITY CALIBRATION
1,2 dichlorobenzene
Liquid Conc., [ppm]
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
0.0
10.0
20.0
30.0
40.0
U.V. Detector Scale
Actual
Calc: r-sq.=

AQUEOUS SOLUBILITY CALIBRATION



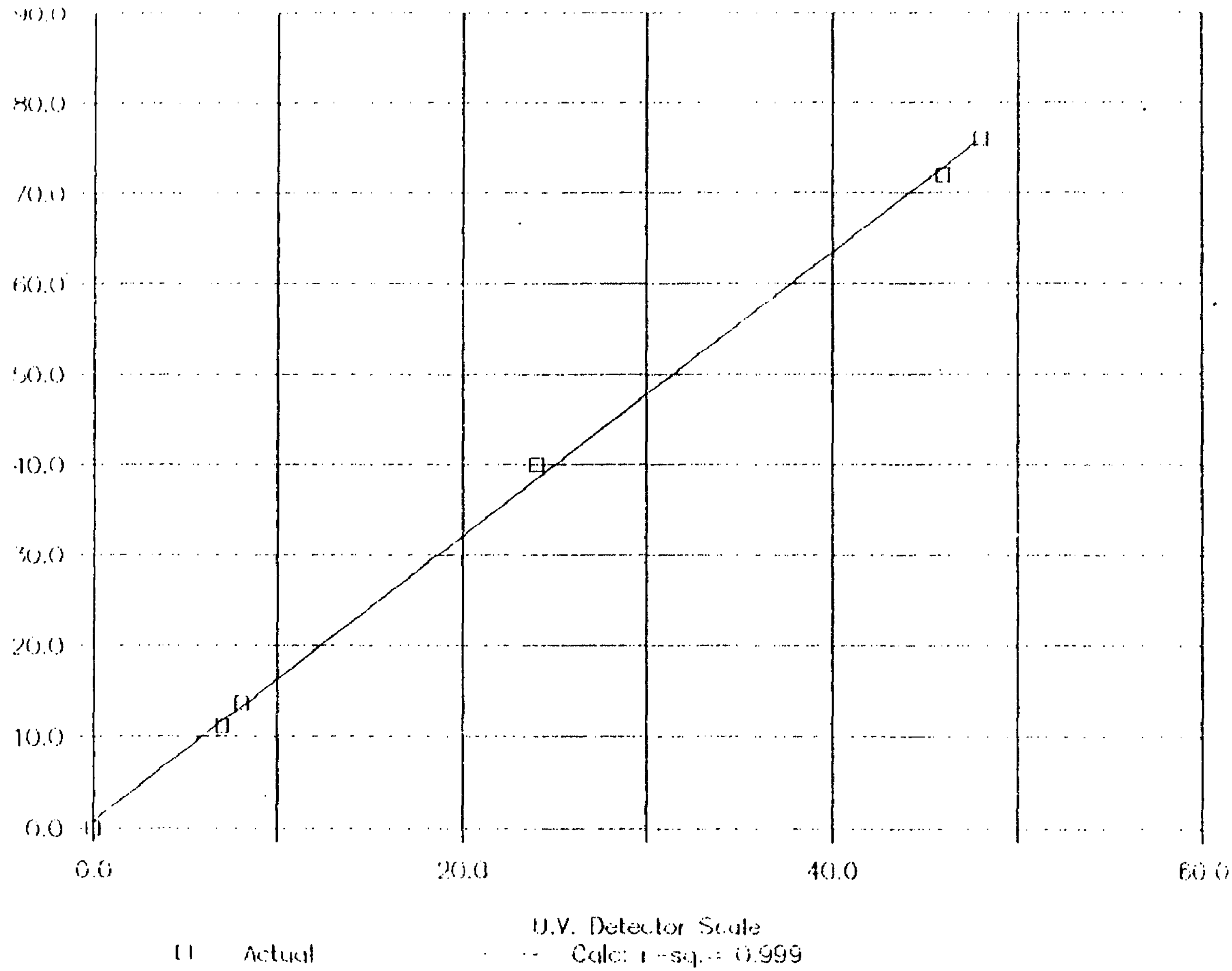
AQUEOUS SOLUBILITY CALIBRATION

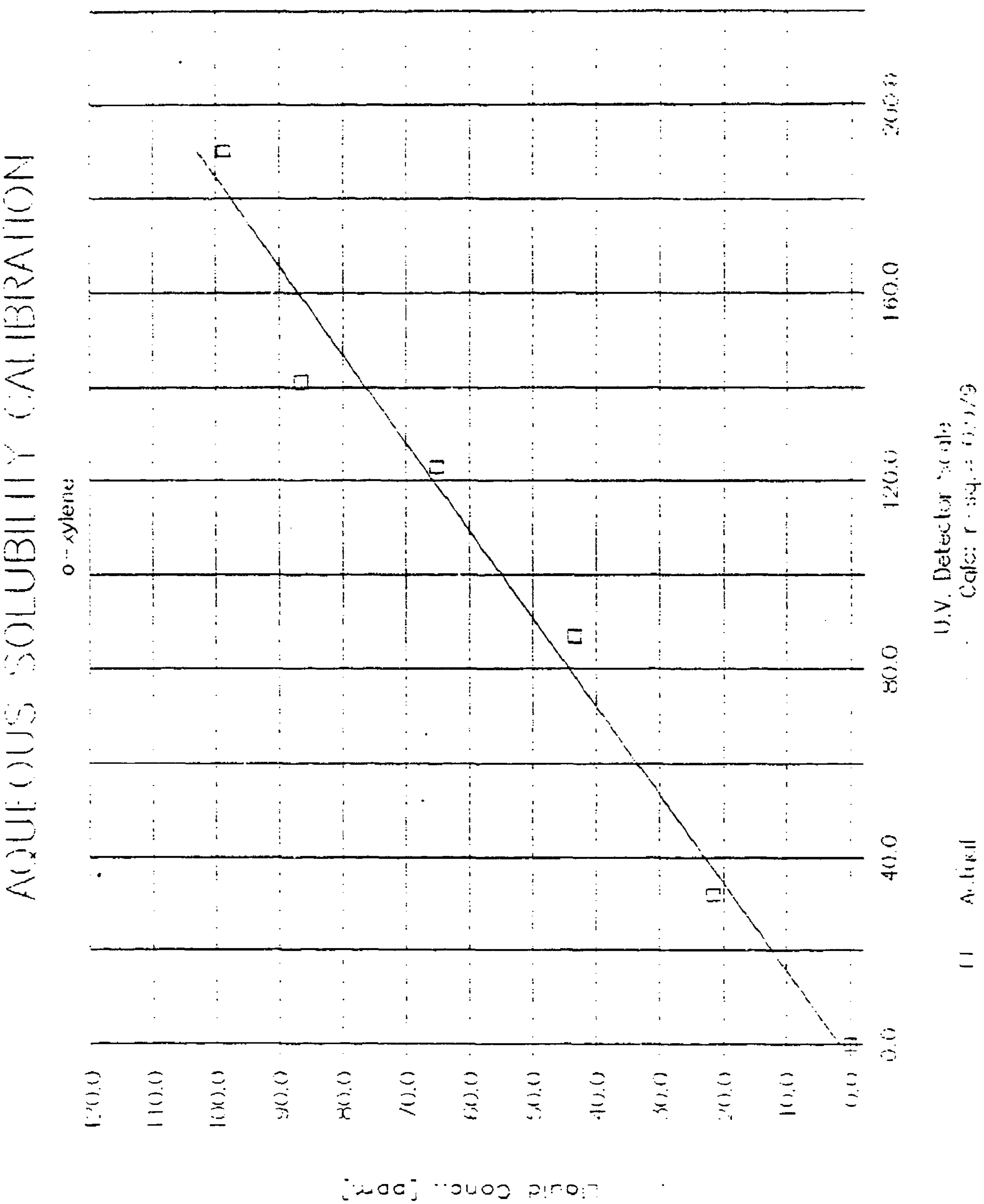
1,3 dichlorobenzene



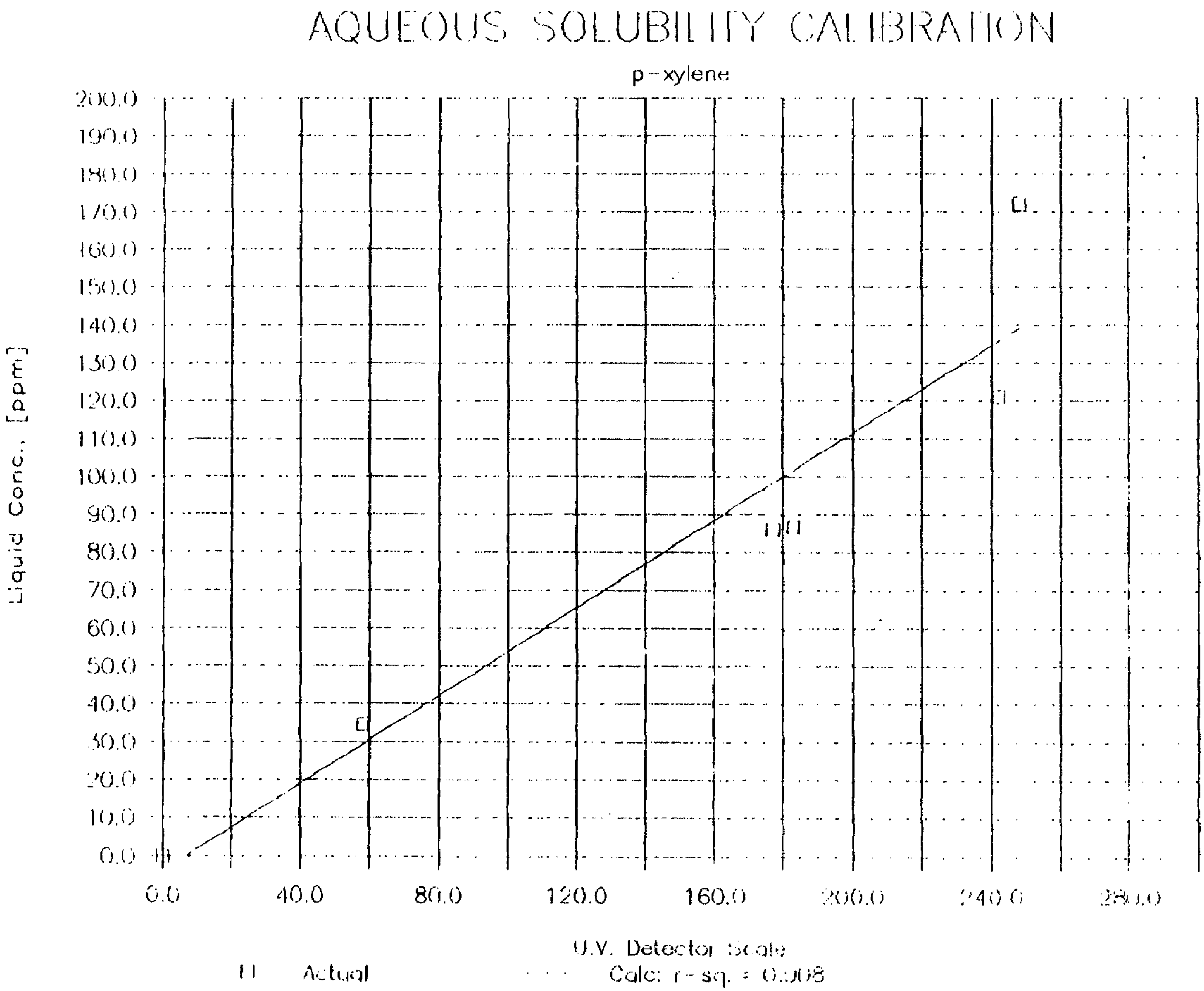
AQUEOUS SOLUBILITY CALIBRATION

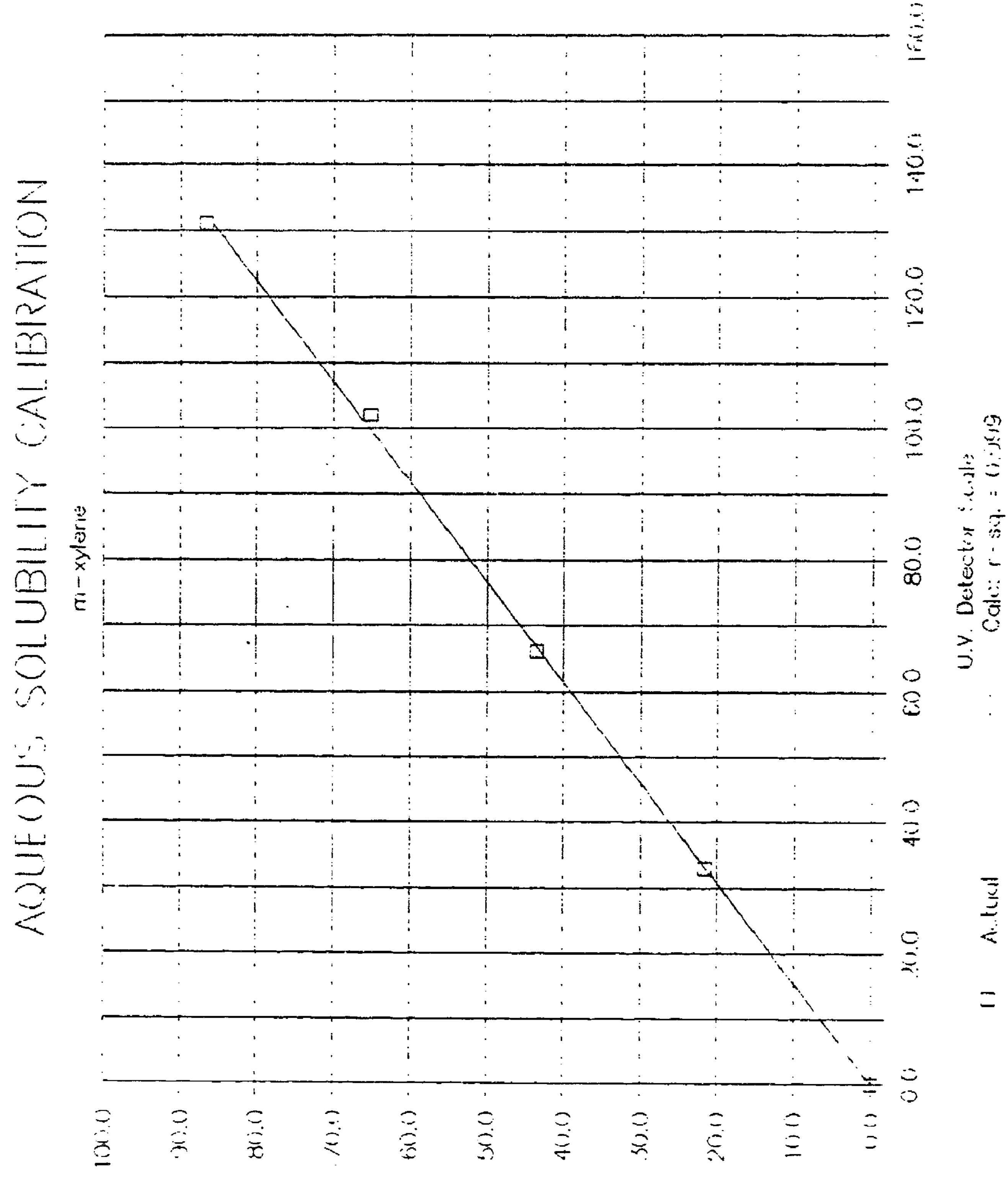
1,4 dichlorobenzene

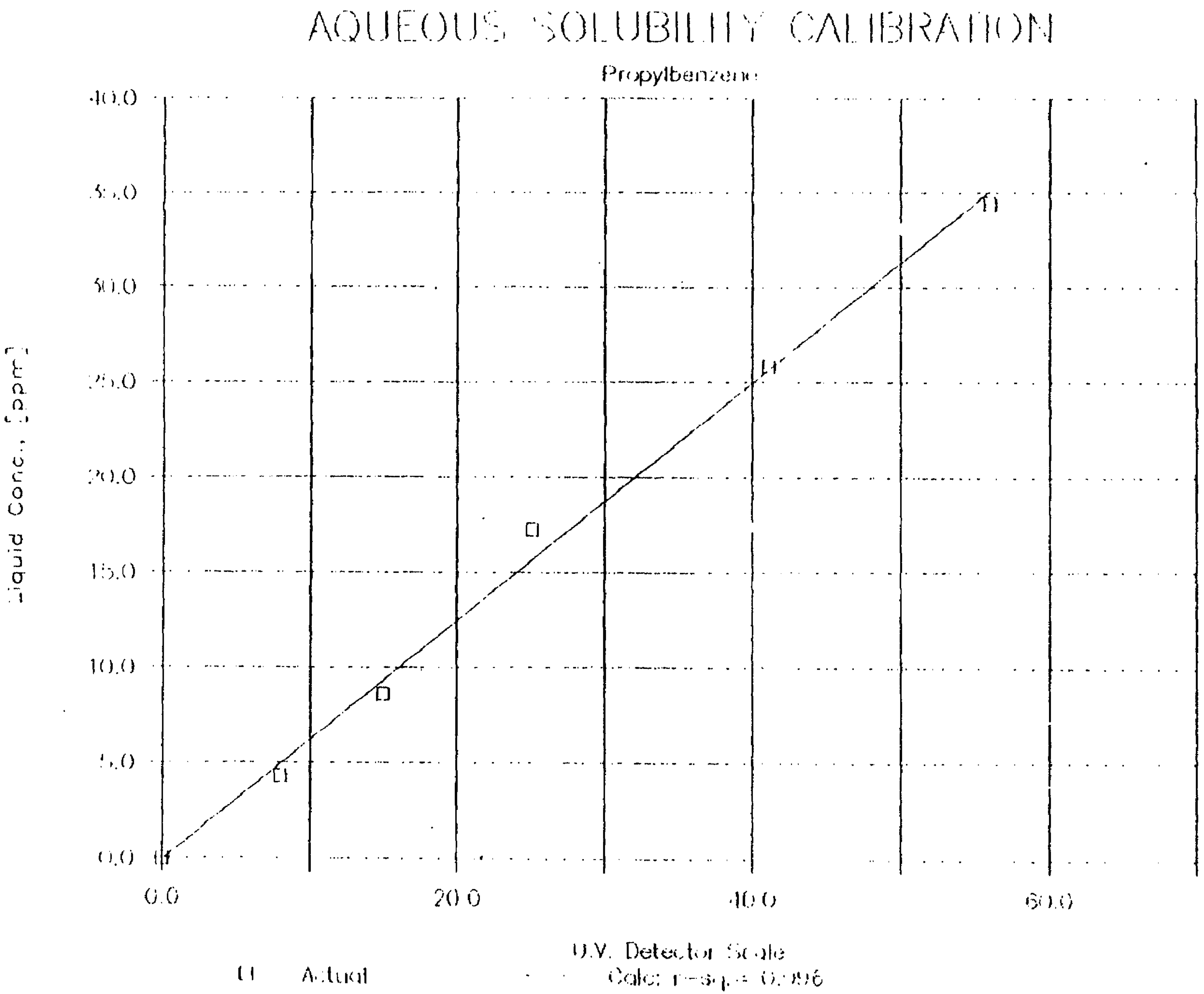


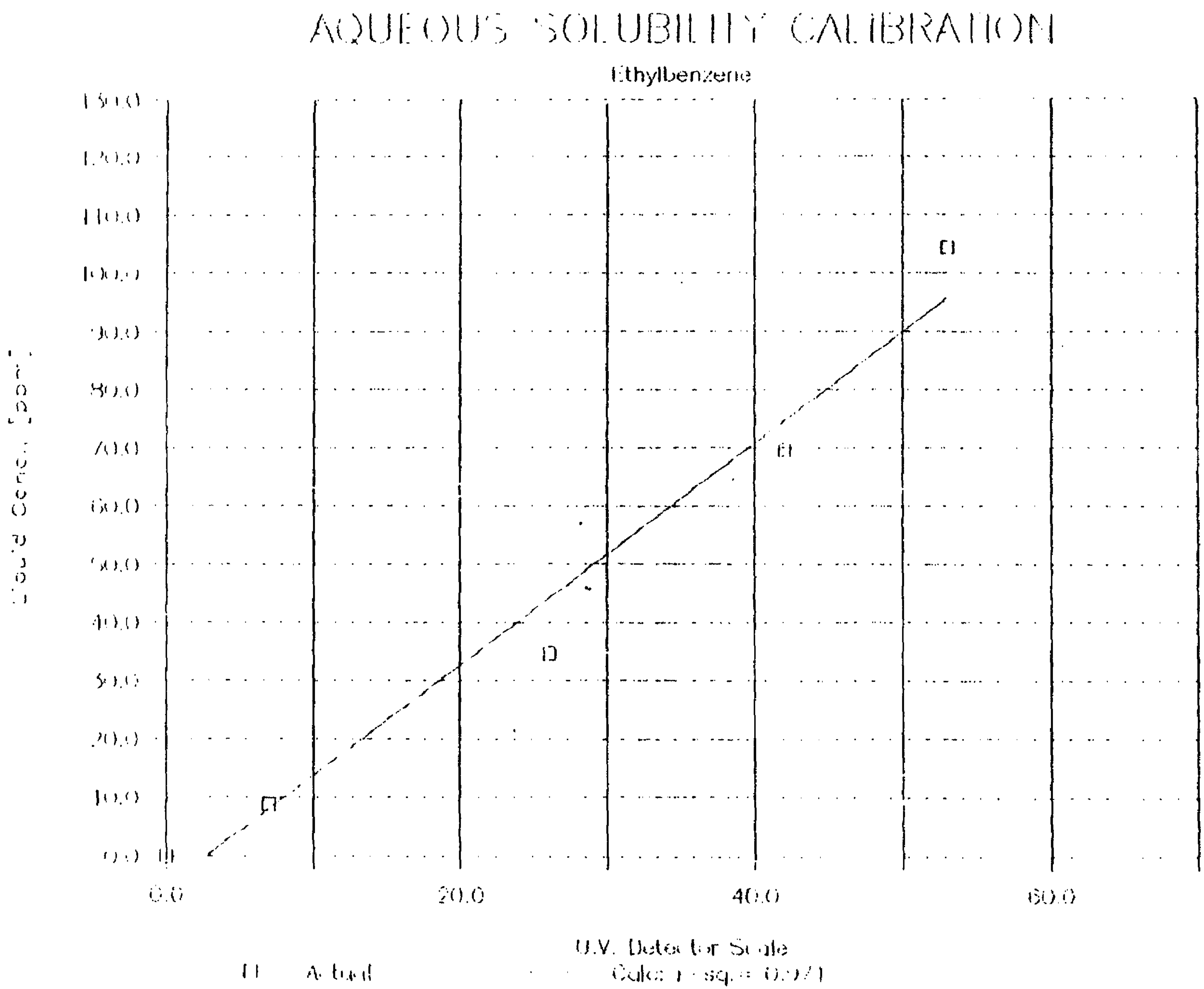


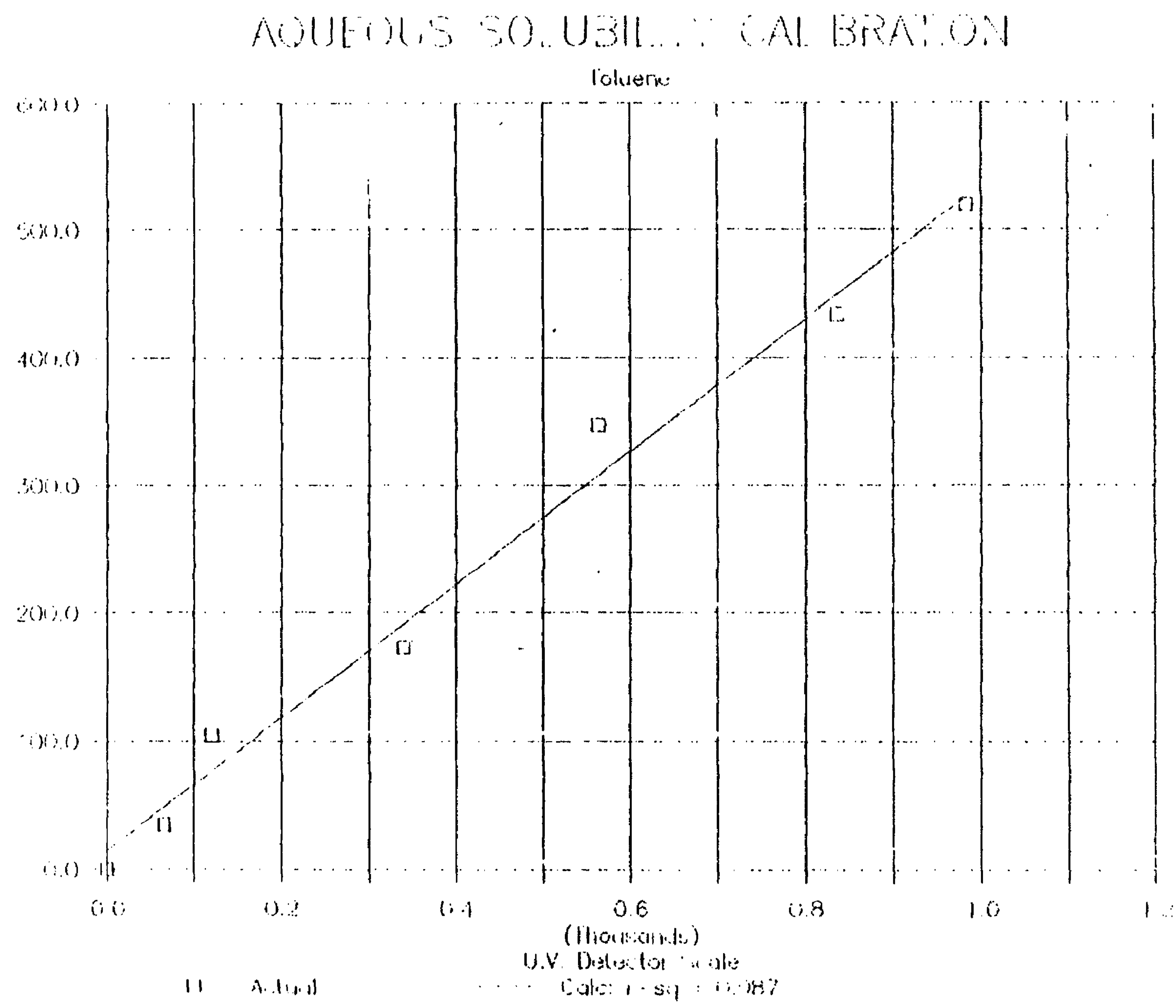
AQUEOUS SOLUBILITY CALIBRATION
o - xylene
0.0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
0.0
40.0
80.0
120.0
160.0
U.V. Detector Scale
Actual


AQUEOUS SOLUBILITY CALIBRATION
p-xylene
Liquid Conc., [ppm]
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
0.0
40.0
80.0
120.0
160.0
200.0
240.0
280.0
U.V. Detector Scale
Actual
Calc: r-sq. = 0.908


AQUEOUS SOLUBILITY CALIBRATION
m-xylene
U.V. Detector Scale
Actual
Liquid Conc. [ppm]
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
10.0
30.0
50.0
70.0
90.0
100.0

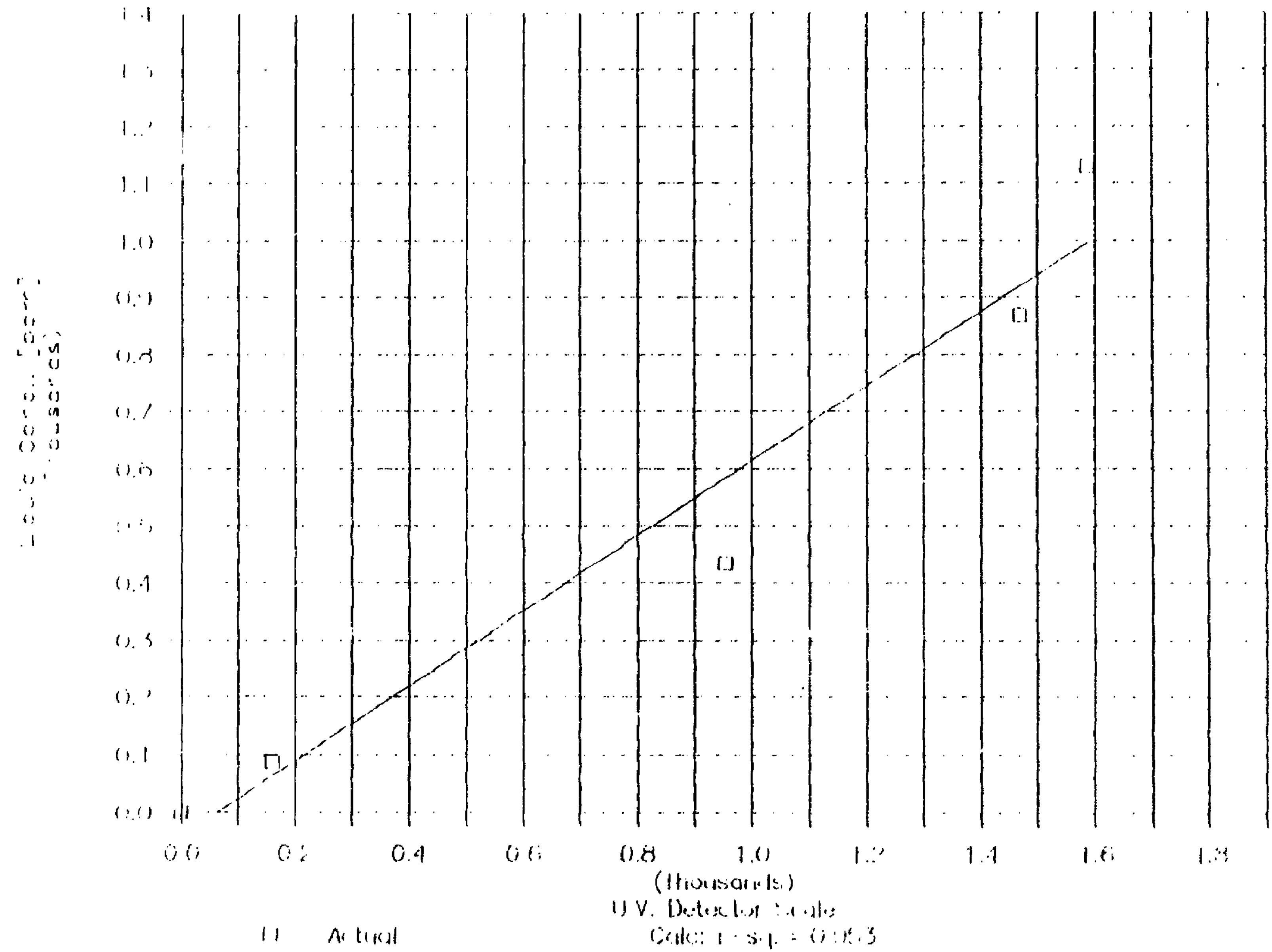

AQUEOUS SOLUBILITY CALIBRATION
Propylbenzene
Liquid Conc., [ppm]
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
0.0
20.0
40.0
60.0
U.V. Detector Scale
Actual

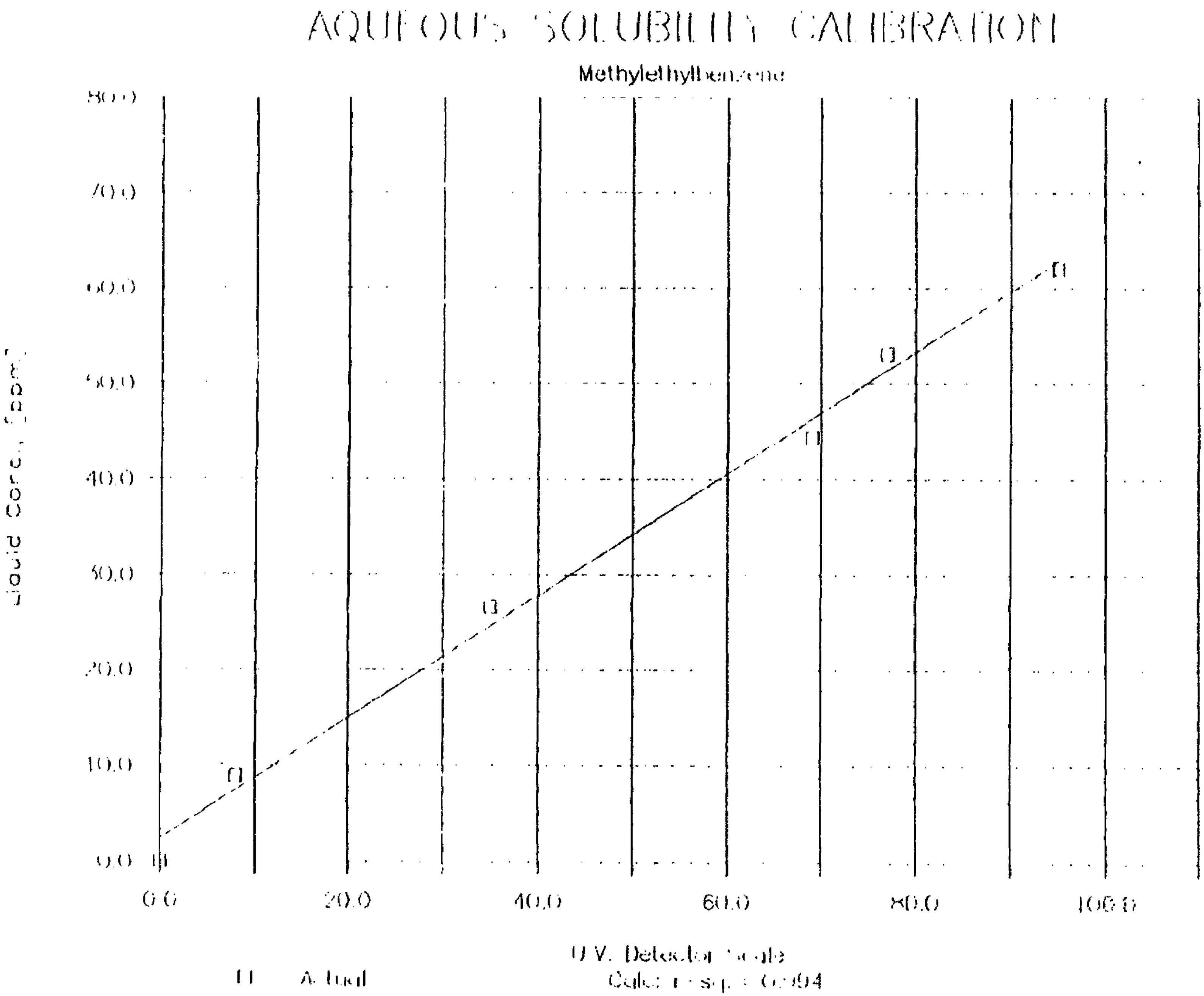

AQUEOUS SOLUBILITY CALIBRATION
Ethylbenzene
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
0.0
20.0
40.0
60.0
U.V. Detector Scale
Actual


AQUEOUS SOLUBILITY CALIBRATION
Toluene
600.0
500.0
400.0
300.0
200.0
100.0
0.0
0.0
0.2
0.4
0.6
0.8
1.0
(Thousands)
U.V. Detector Scale
Actual
Calc

AQUEOUS SOLUBILITY CALIBRATION

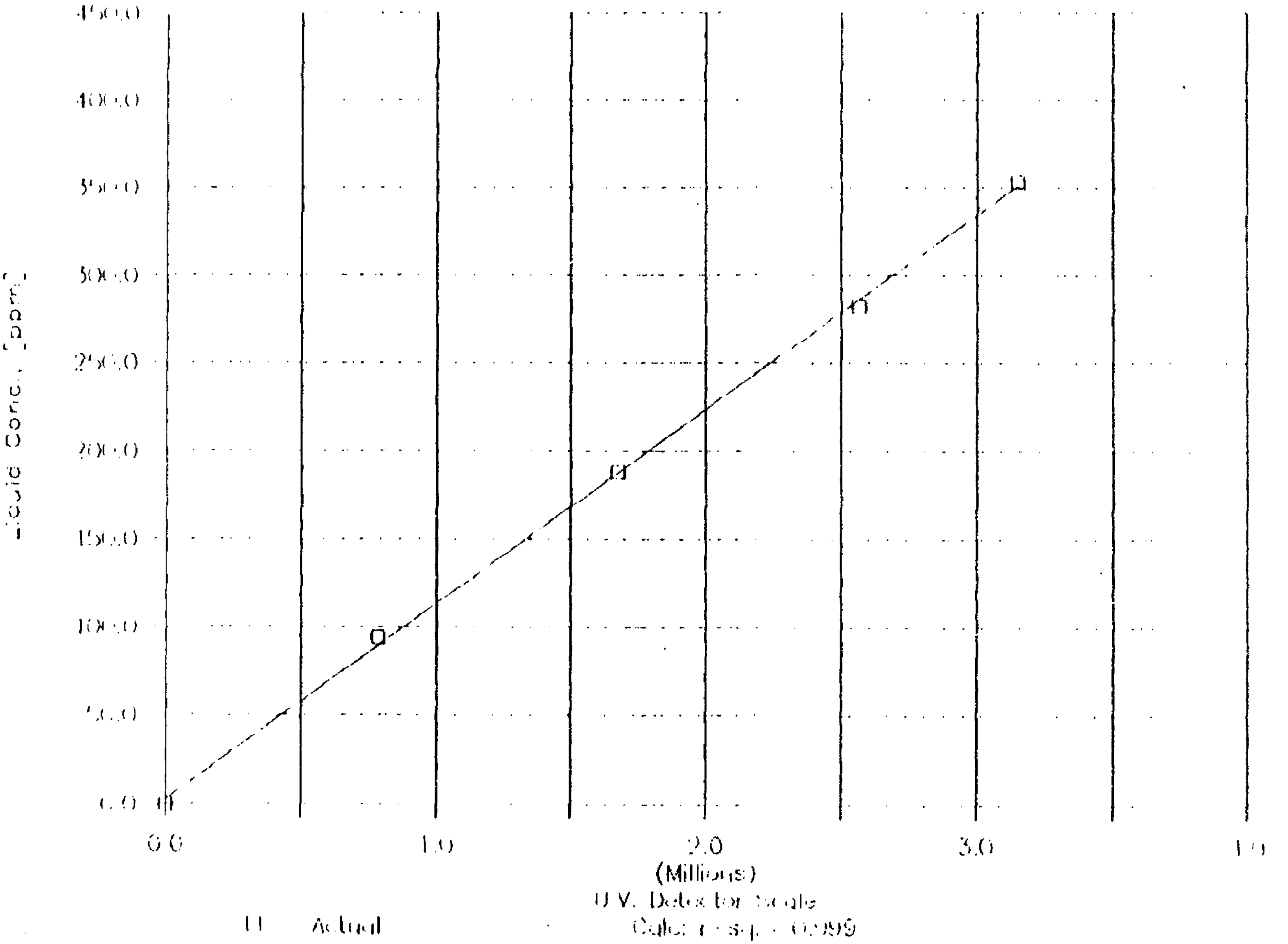
Benzene

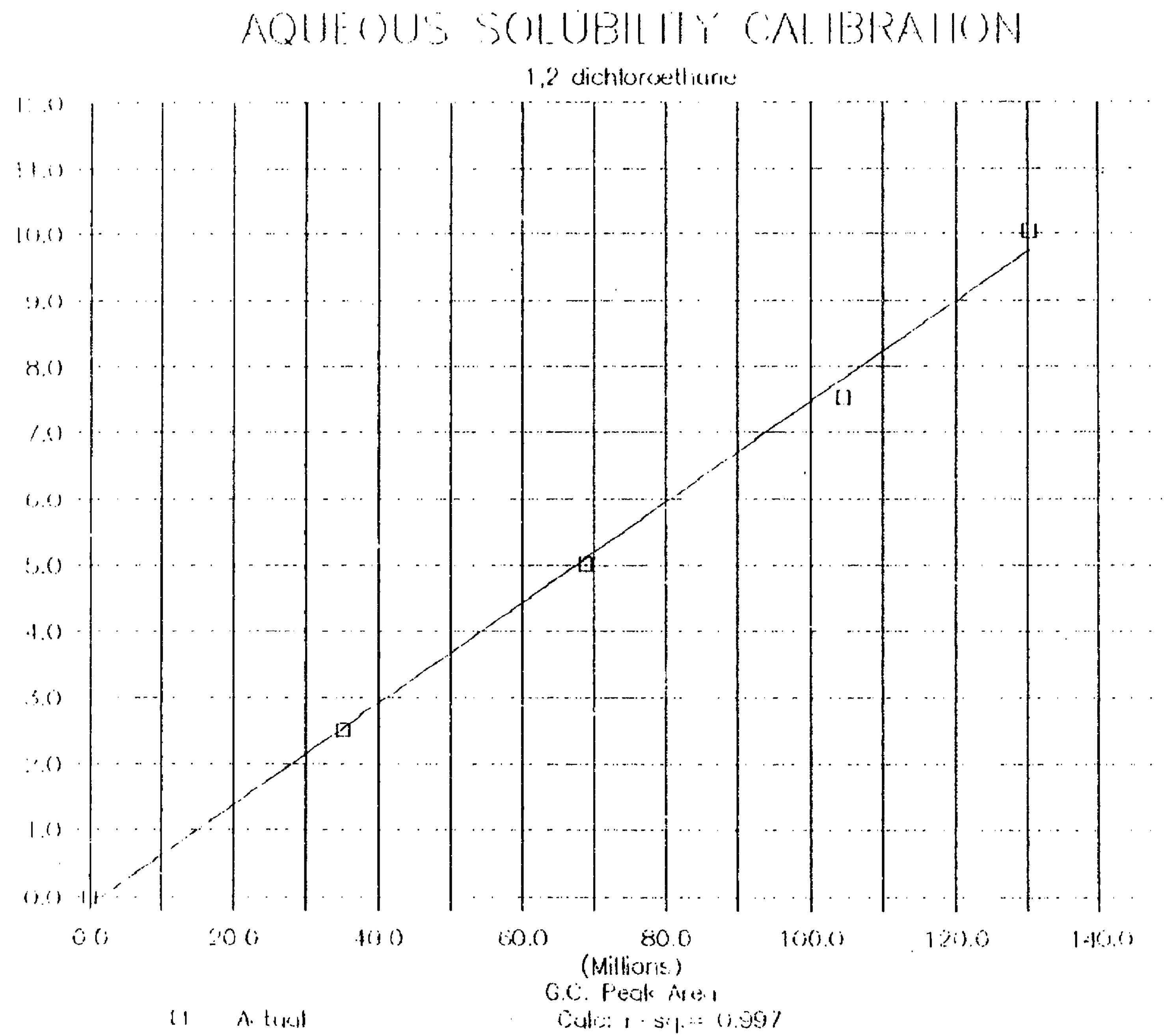


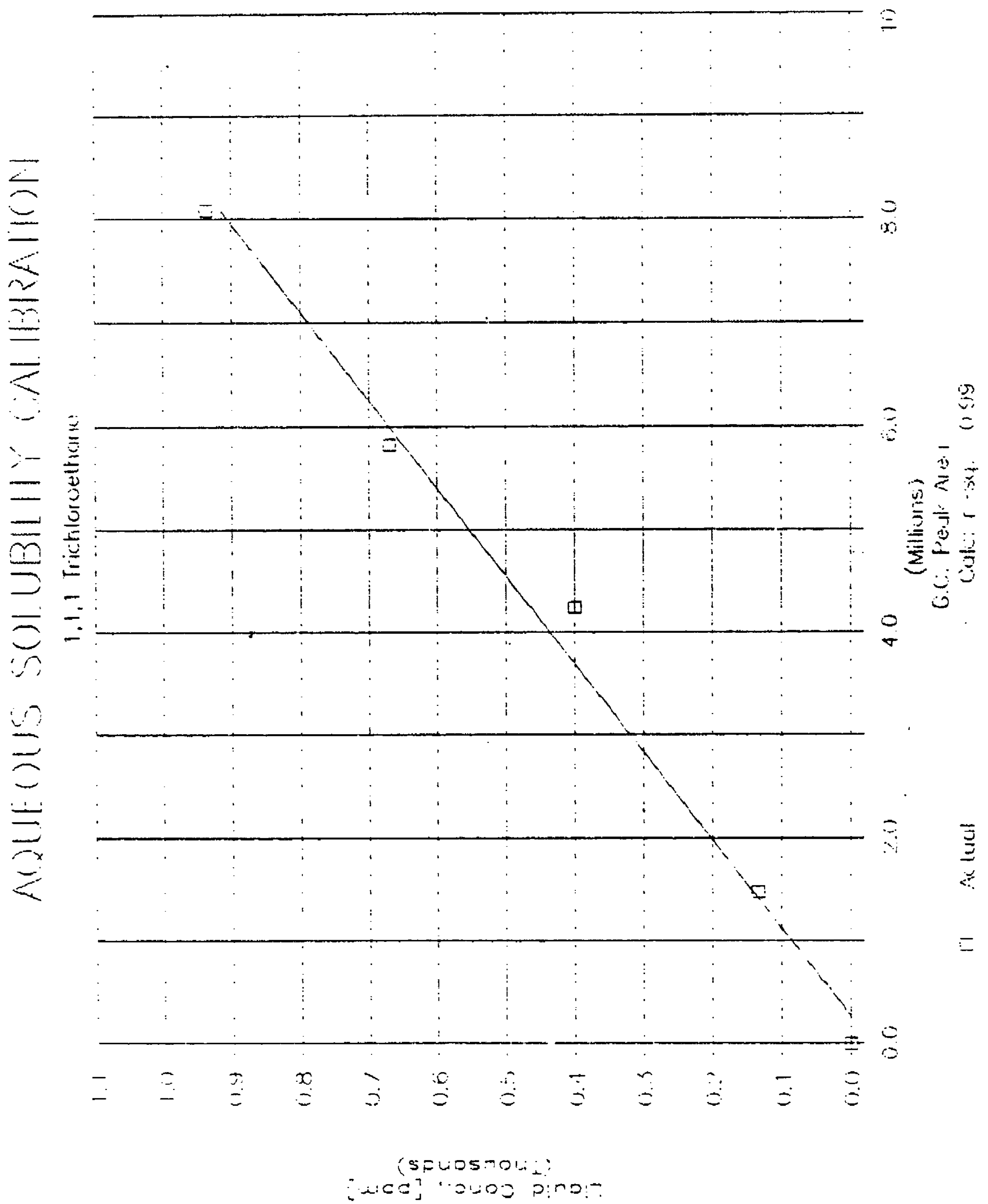

AQUEOUS SOLUBILITY CALIBRATION
Methylethylbenzene
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
0.0
20.0
40.0
60.0
80.0
U.V. Detector Scale
Actual

AQUEOUS SOLUBILITY CALIBRATION

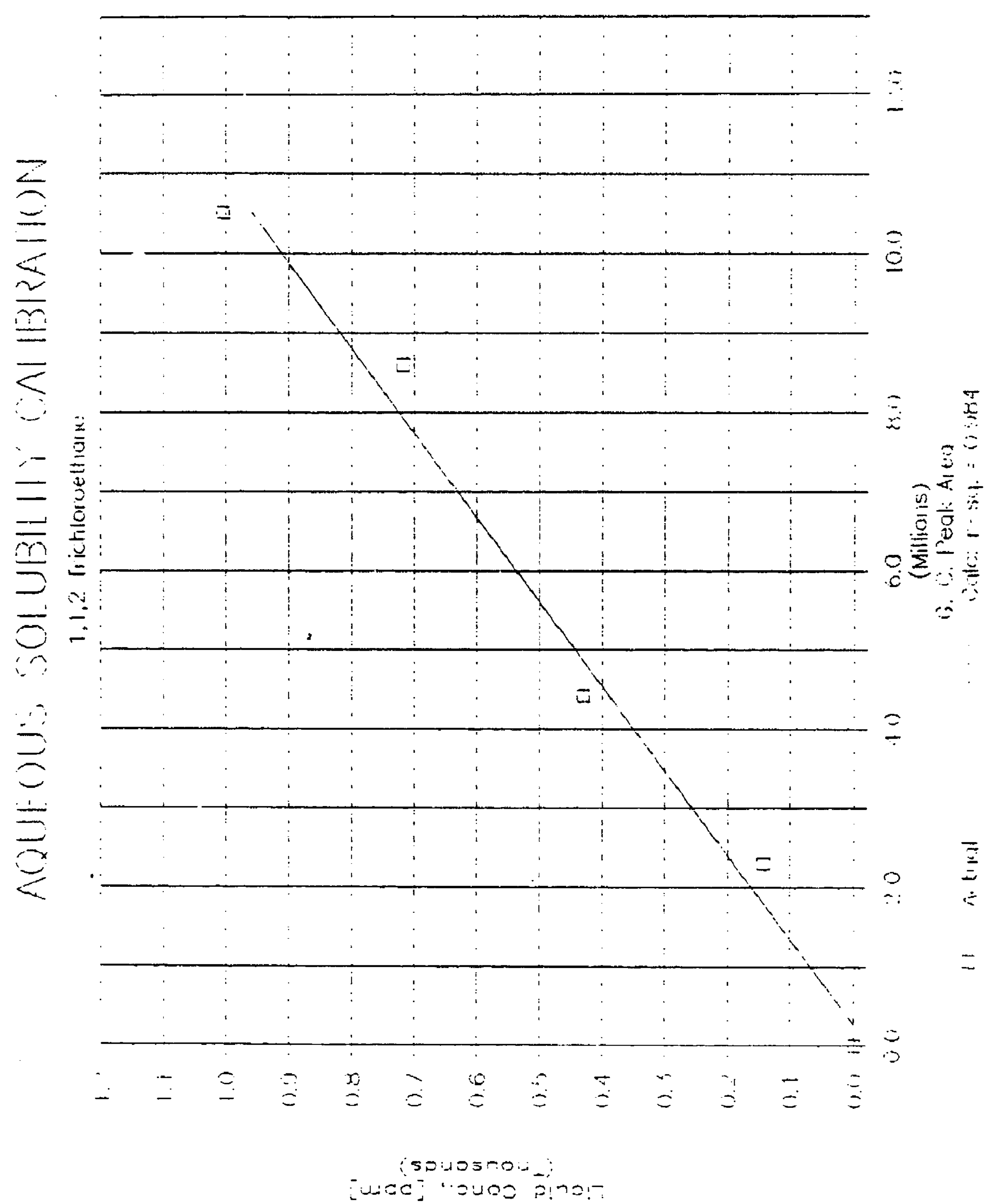
1,1 dichloroethane

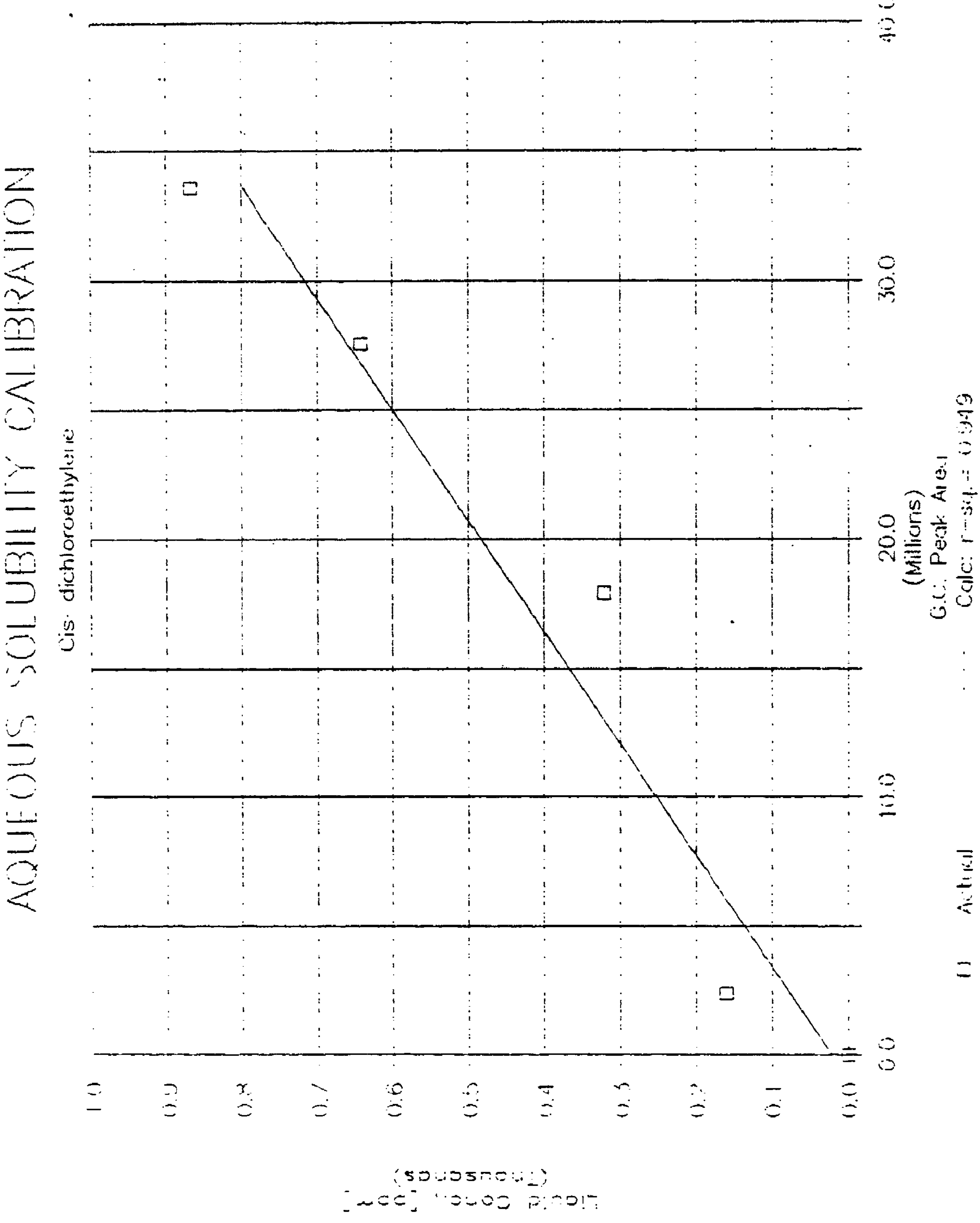



AQUEOUS SOLUBILITY CALIBRATION
1,2 dichloroethane
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
(Millions)
G.C. Peak Area
□ Actual
Calc: r-sq = 0.997



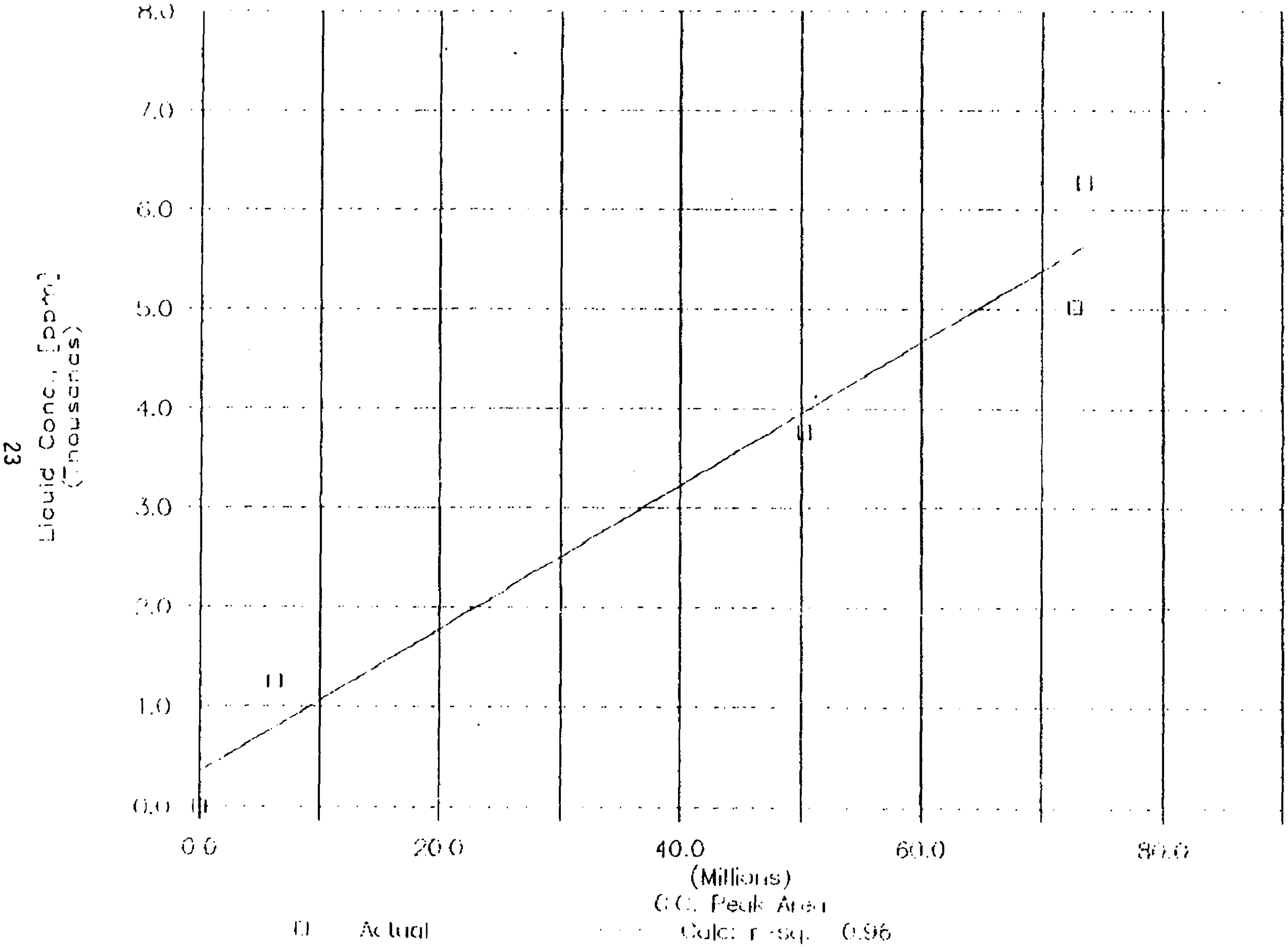
AQUEOUS SOLUBILITY CALIBRATION
1,1,1 Trichloroethane
Liquid Conc. [ppm]
(Thousands)
(Millions)
G.C. Peak Area
Actual
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
2.0
4.0
6.0
8.0

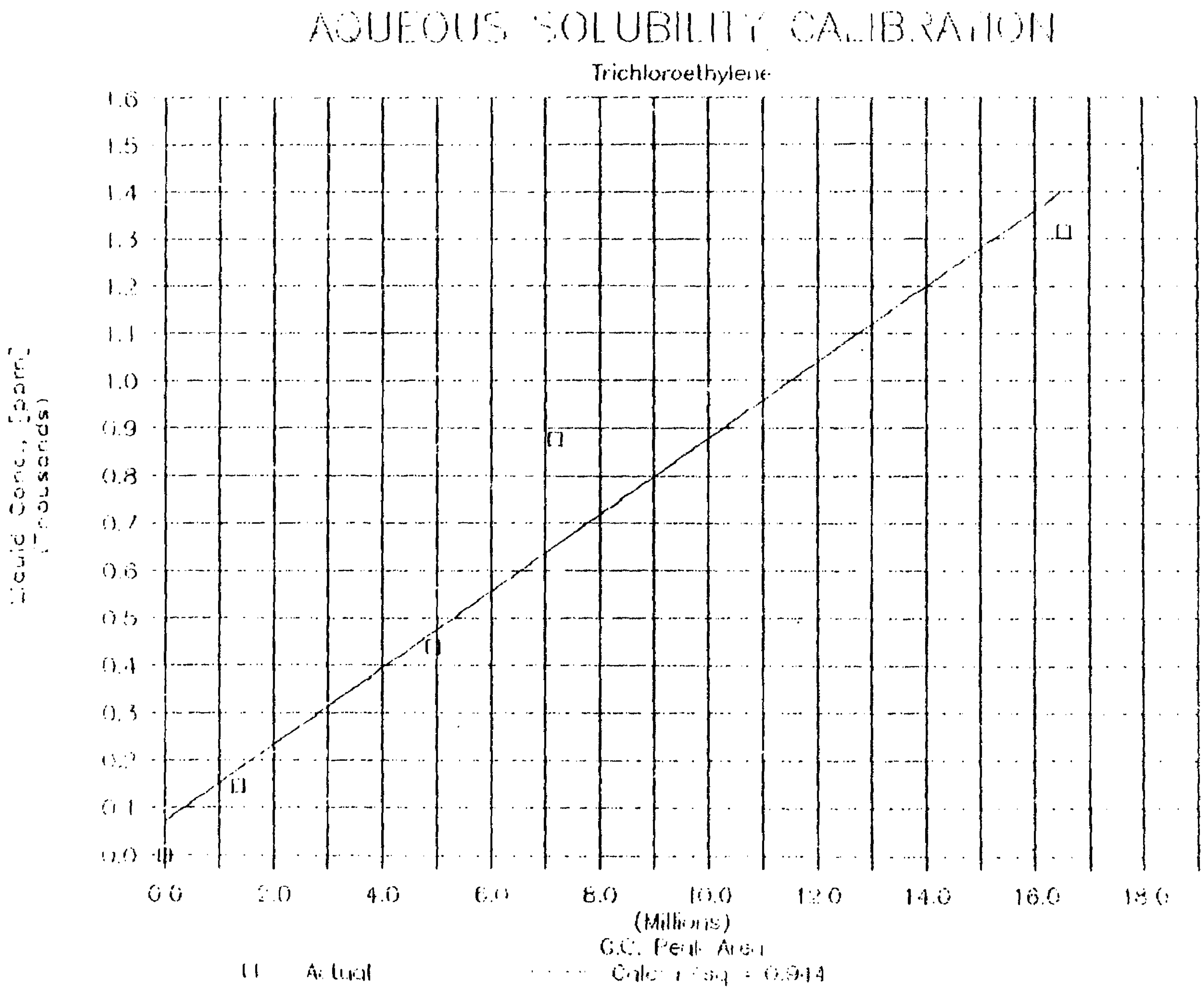

AQUEOUS SOLUBILITY CALIBRATION
1,1,2 Trichloroethane
Liquid Conc. [ppm]
(Thousands)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0.0
2.0
4.0
6.0
8.0
10.0
(Millions)
G. C. Peak Area
Actual


AQUEOUS SOLUBILITY CALIBRATION
Cis dichloroethylene
Liquid Concn [ppm]
(Thousands)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
0.0
10.0
20.0
30.0
40.0
(Millions)
G.C. Peak Area
□ Actual
Calc: r-sq = 0.949

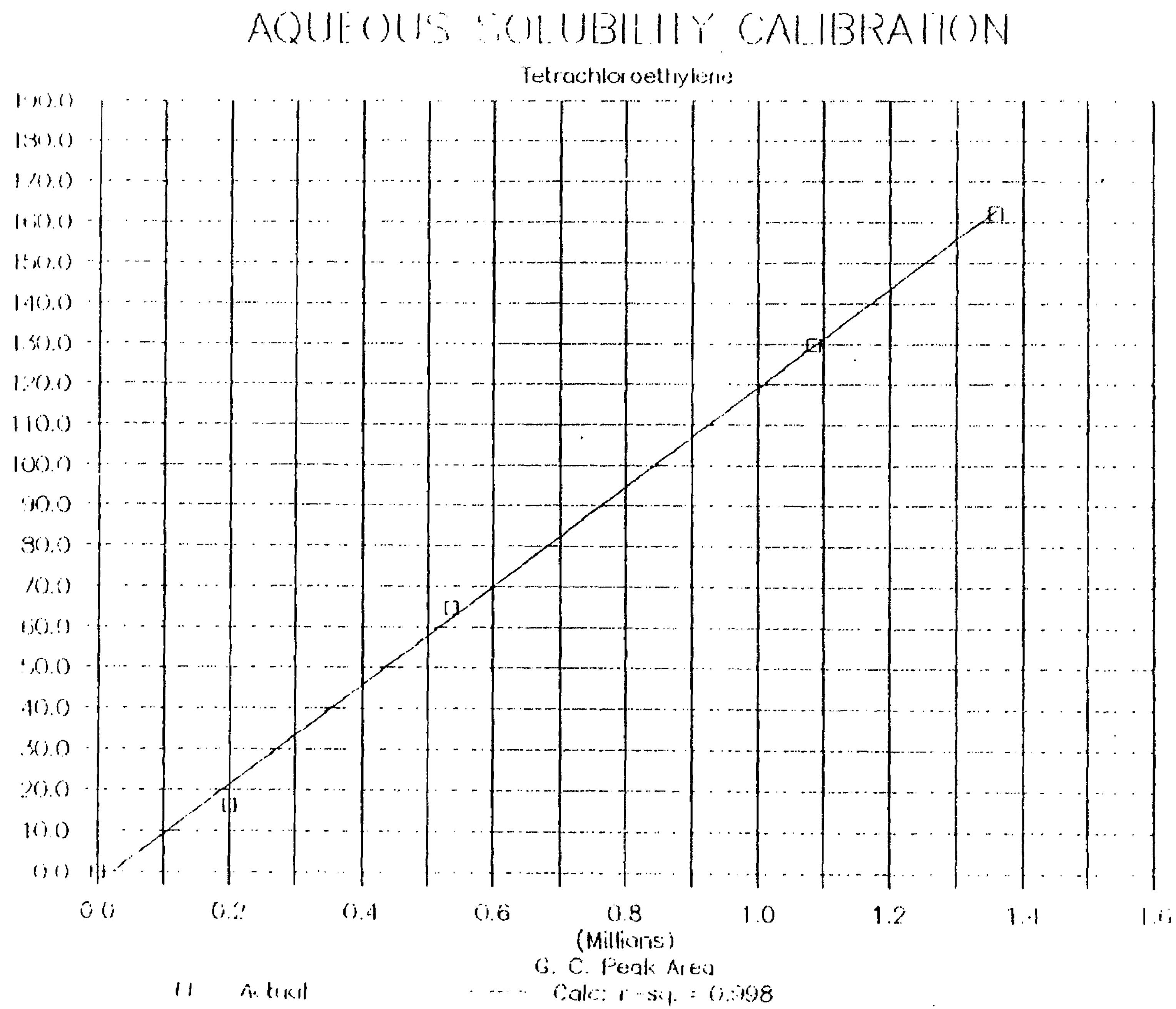
AQUEOUS SOLUBILITY CALIBRATION

trans-dichloroethylene



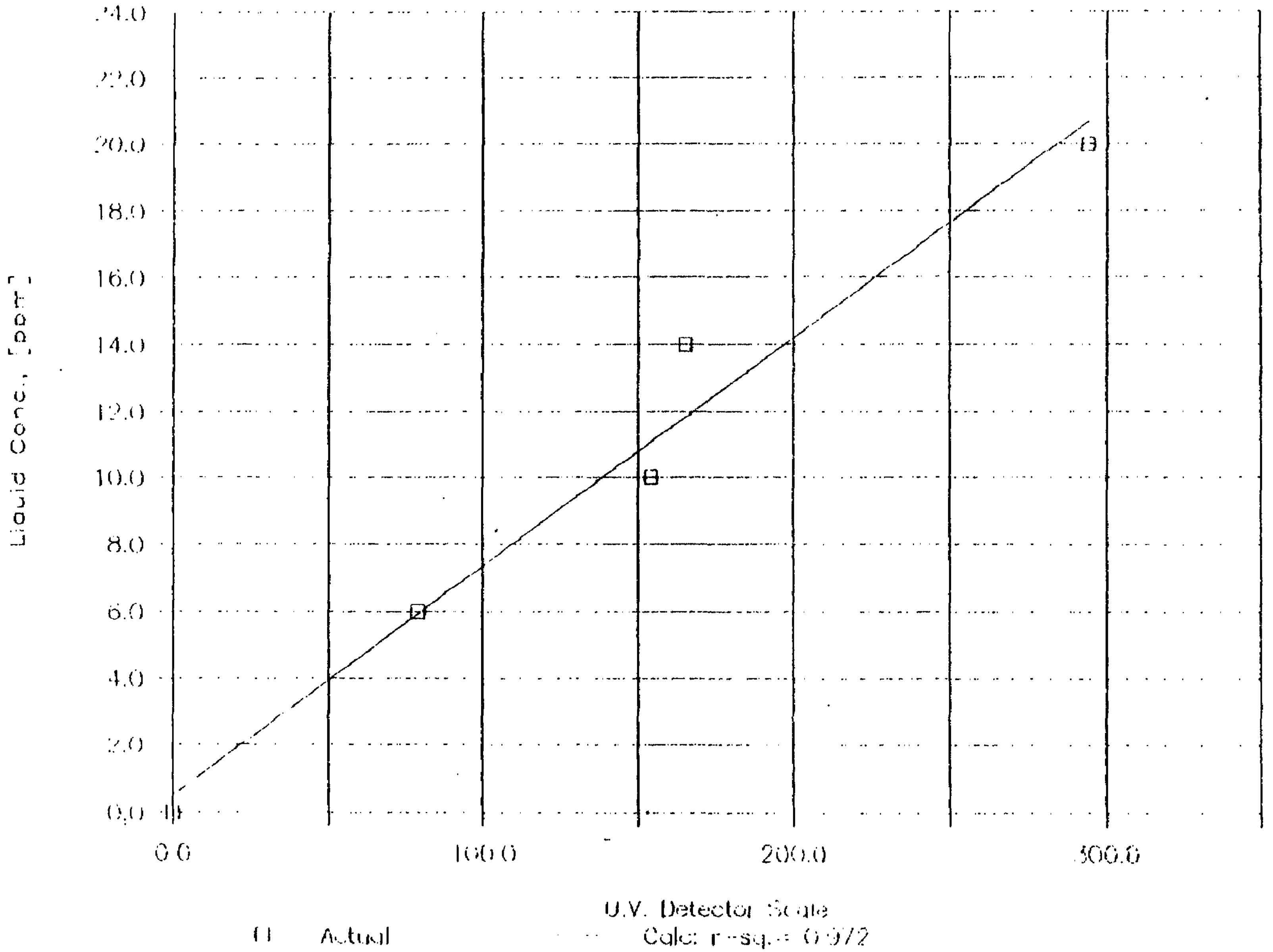


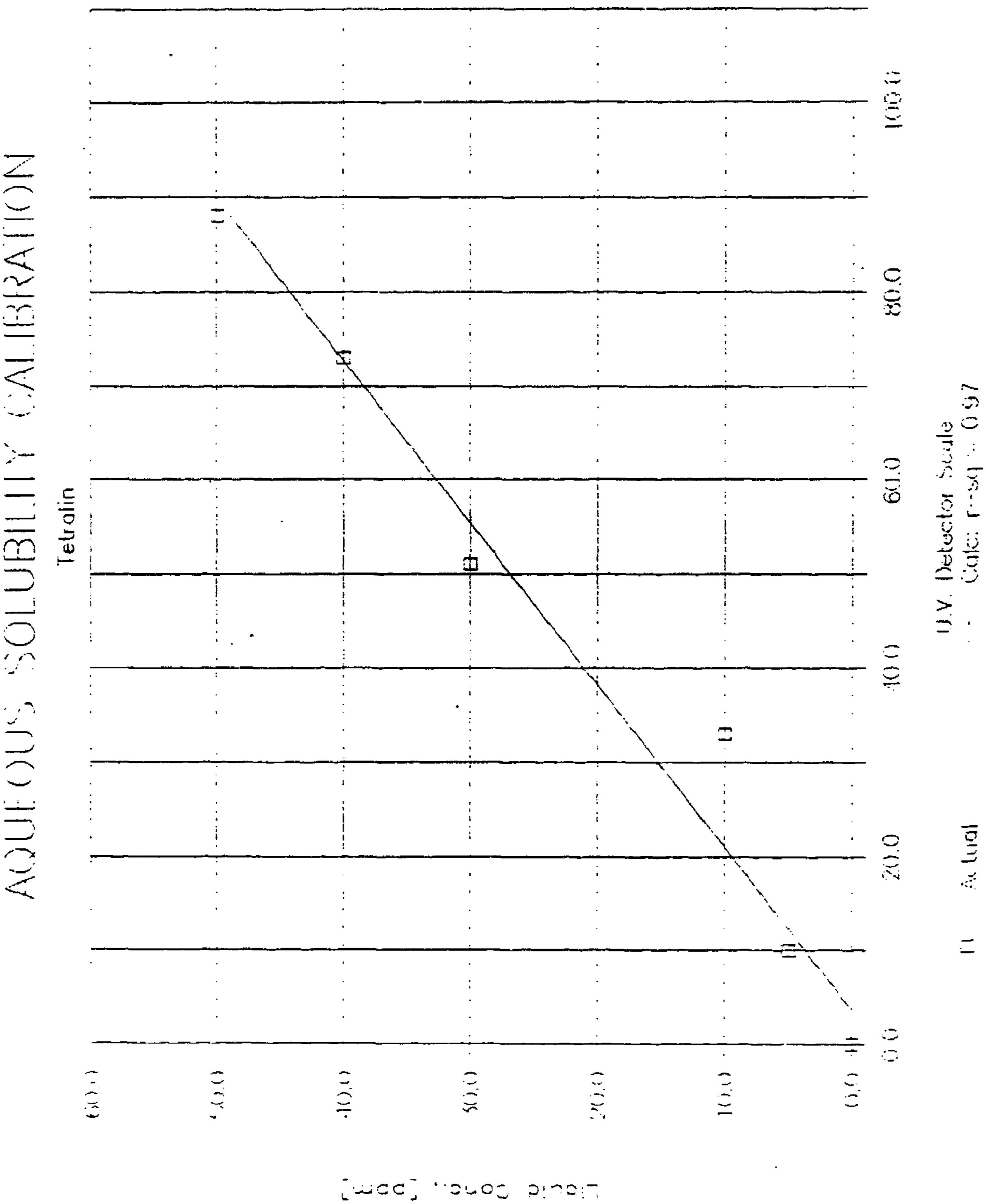
AQUEOUS SOLUBILITY CALIBRATION
Trichloroethylene
Liquid Conc., [ppm]
(Thousands)
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
(Millions)
G.C. Peak Area
Actual
Calc r-sq = 0.944


AQUEOUS SOLUBILITY CALIBRATION
Tetrachloroethylene
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
(Millions)
G. C. Peak Area
Actual
Calc: r-sq. = 0.998

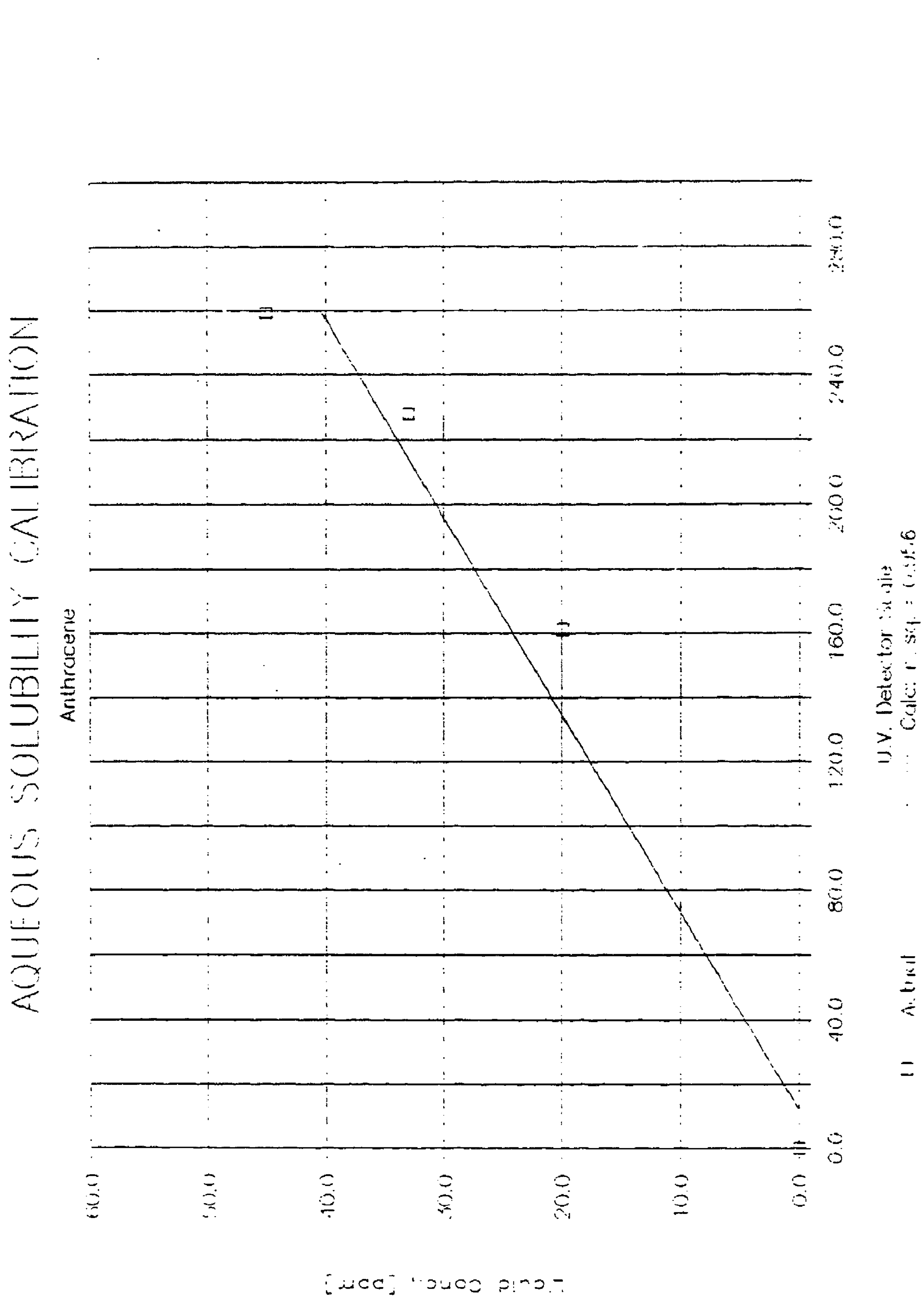
AQUEOUS SOLUBILITY CALIBRATION

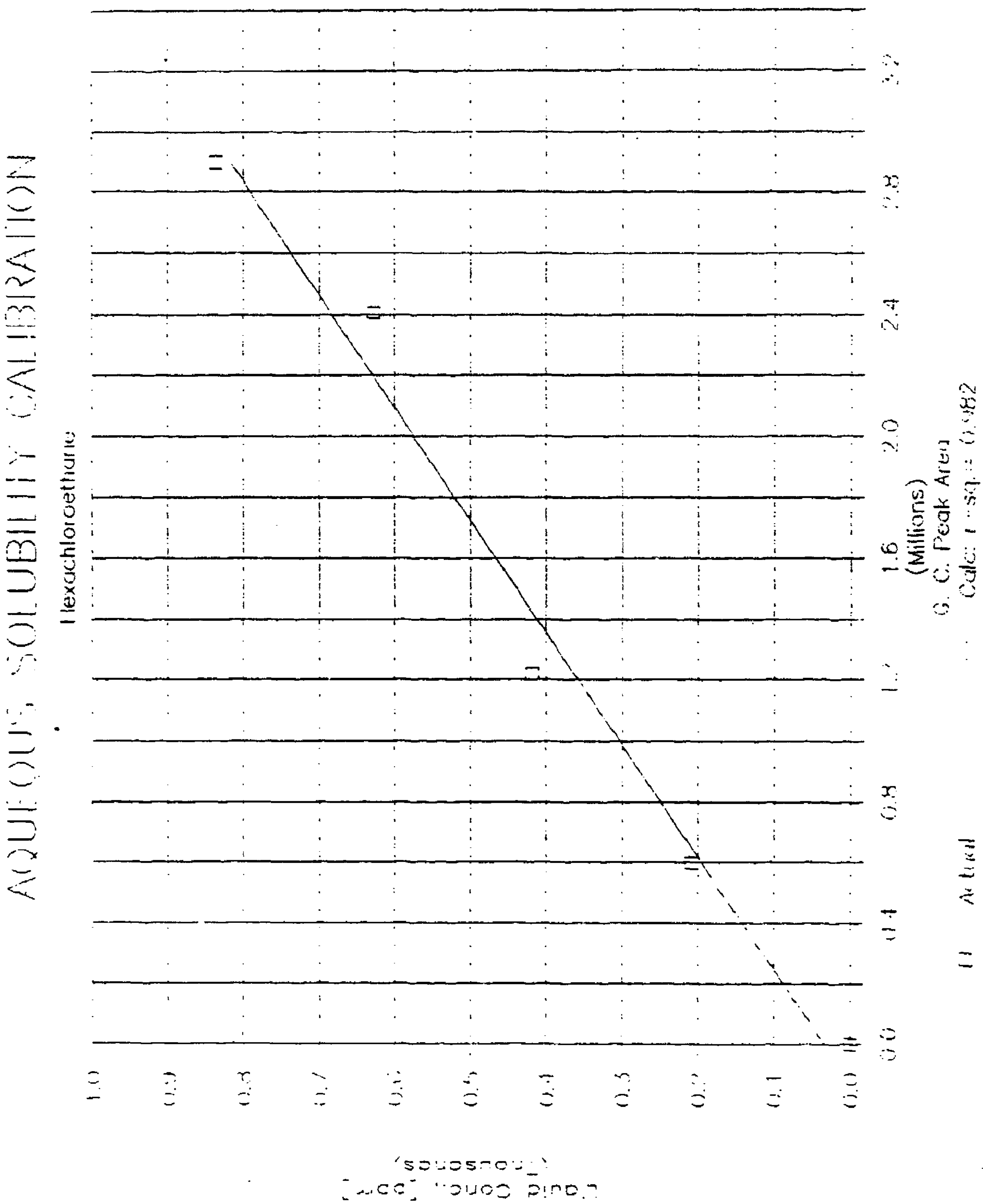
Napthalene





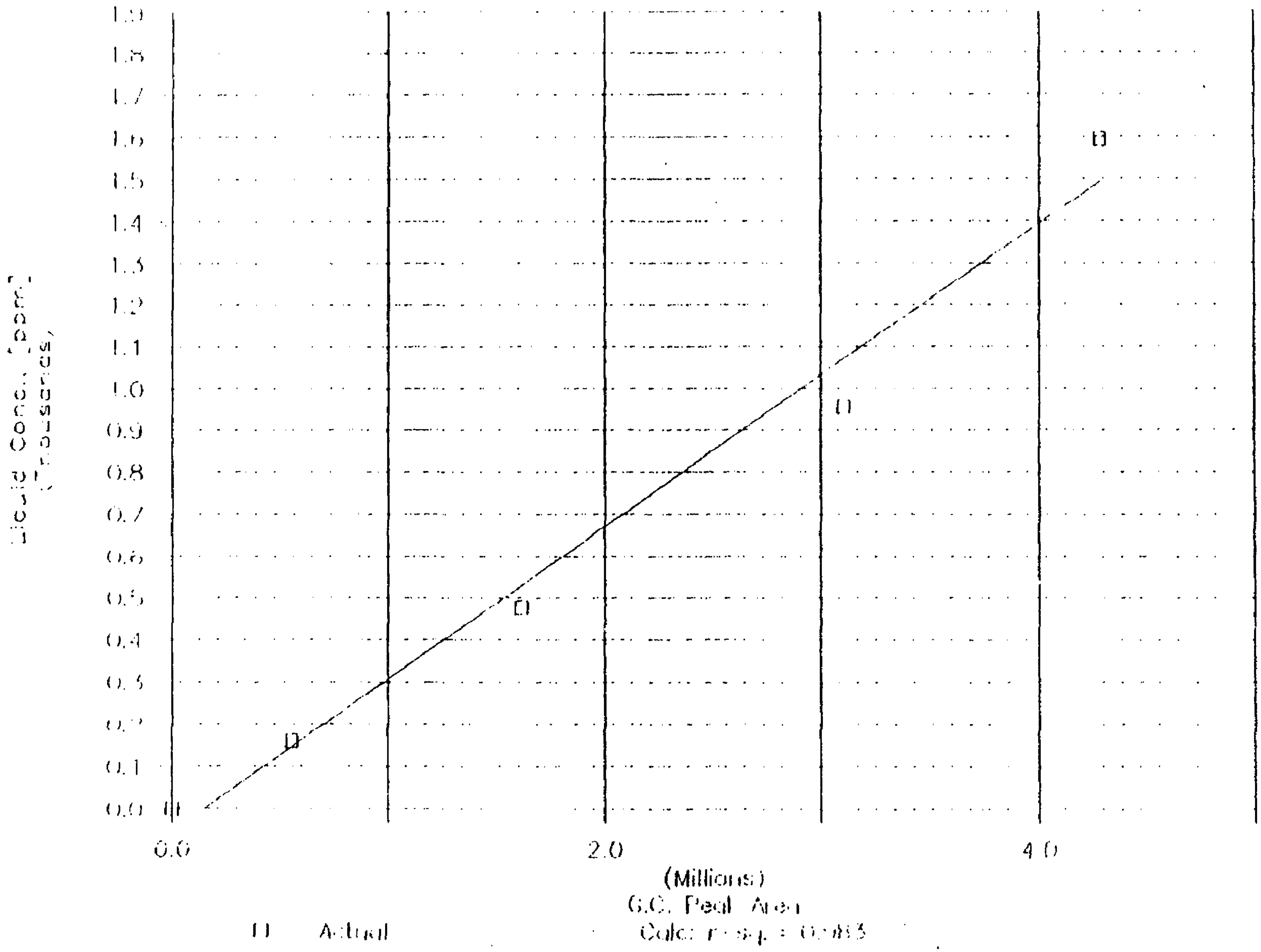
AQUEOUS SOLUBILITY CALIBRATION
Tetralin
U.V. Detector Scale
Calc: r-sq = 0.97
□ Actual
0.0
20.0
40.0
60.0
80.0
100.0
0.0
10.0
20.0
30.0
40.0
50.0
60.0
Liquid Conc. [ppm]

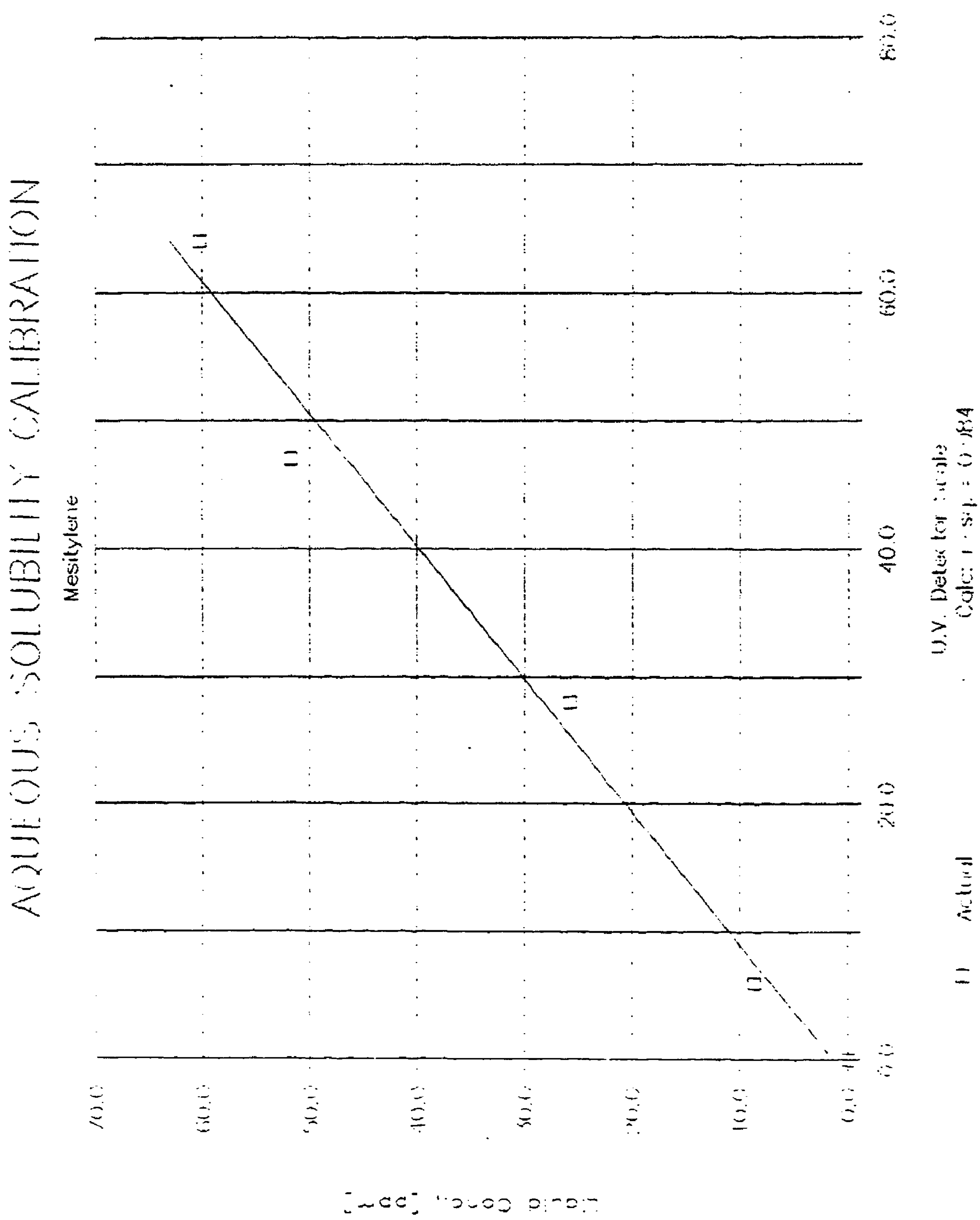

AQUEOUS SOLUBILITY CALIBRATION
Anthracene
0.0
10.0
20.0
30.0
40.0
50.0
60.0
0.0
40.0
80.0
120.0
160.0
200.0
240.0
U.V. Detector Scale
Actual


AQUEOUS SOLUBILITY CALIBRATION
Hexachloroethane
Liquid Conc. [ppm]
(Thousands)
1.6
2.0
2.4
(Millions)
G. C. Peak Area
Actual

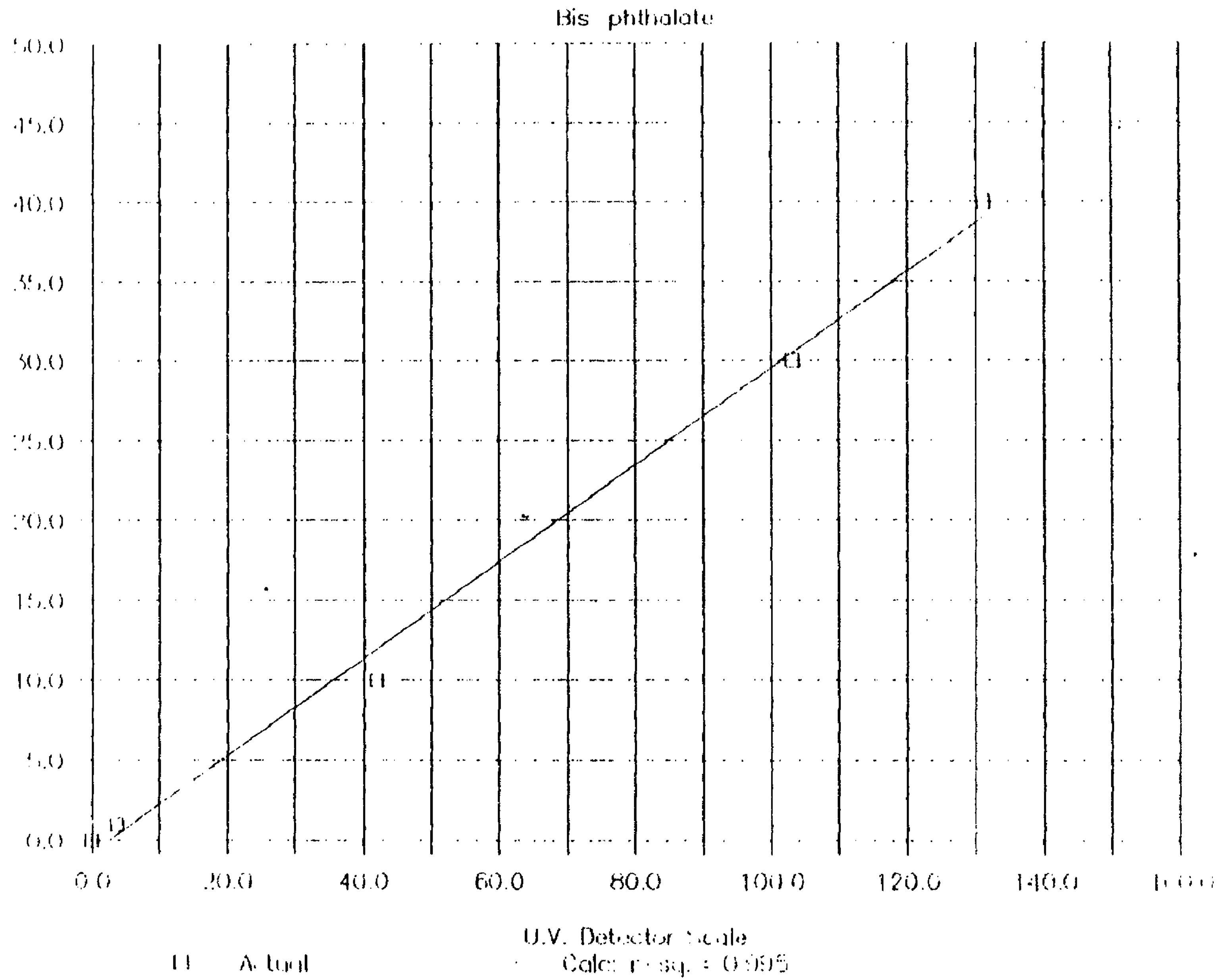
AQUEOUS SOLUBILITY CALIBRATION

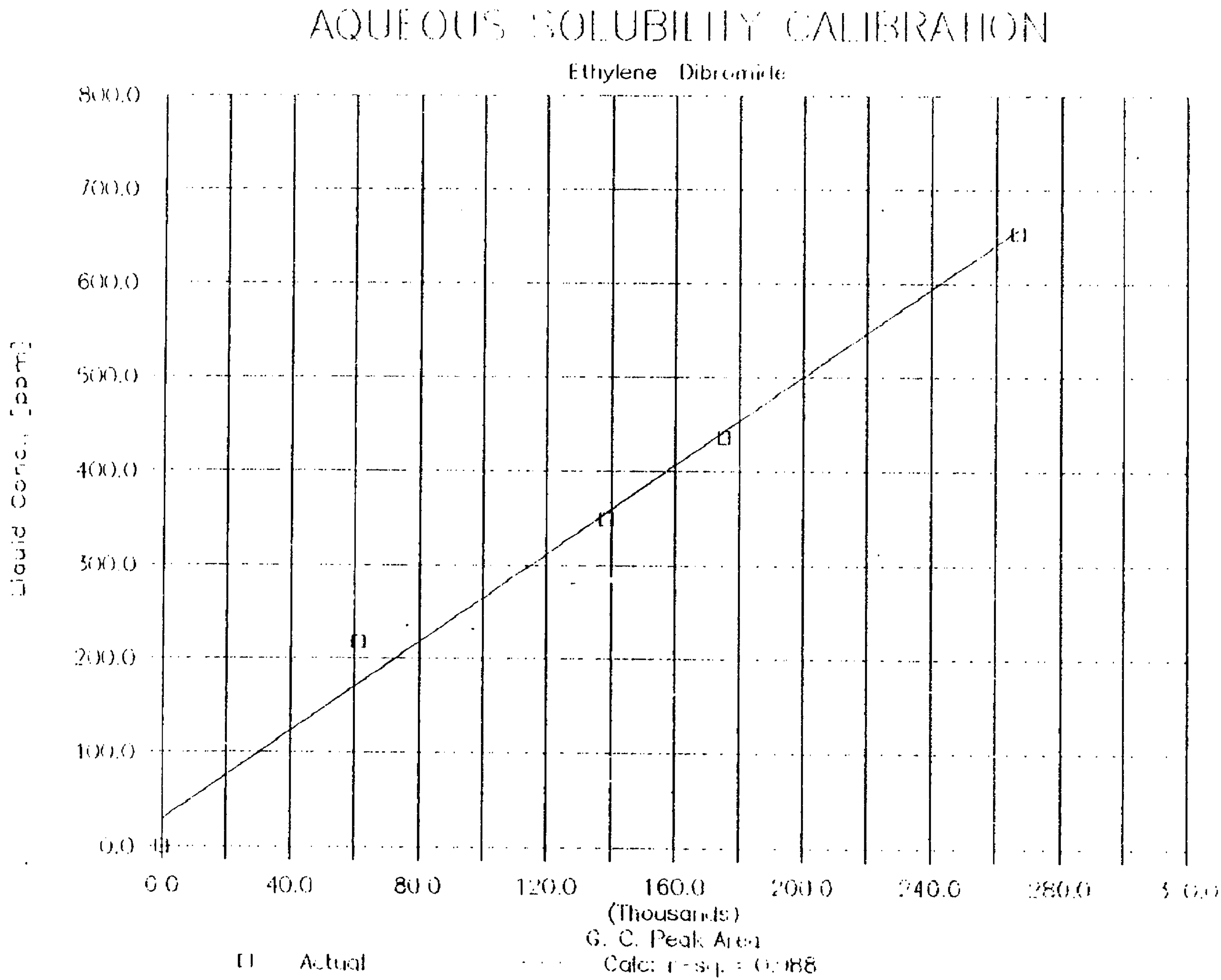
Carbon Tetrachloride

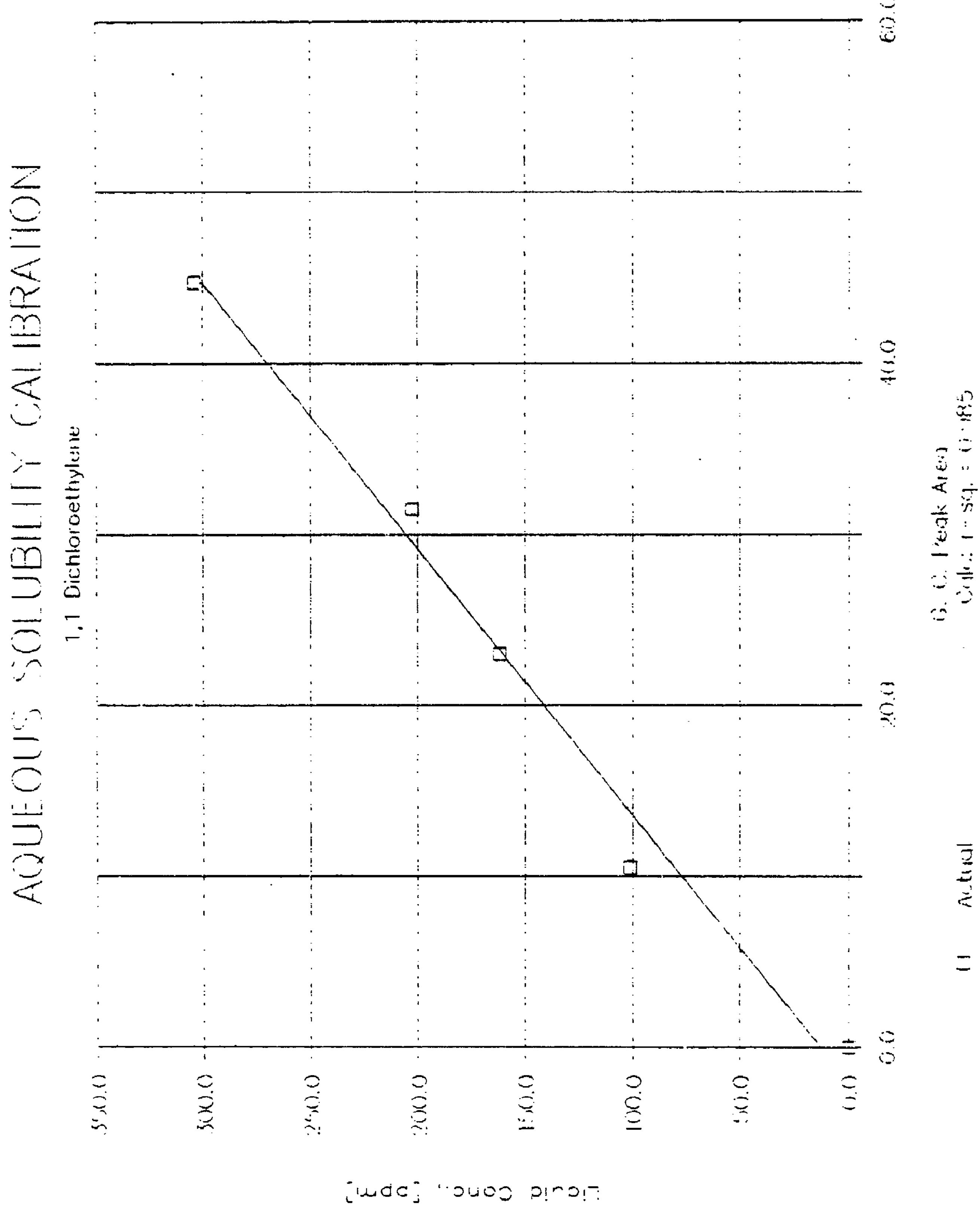


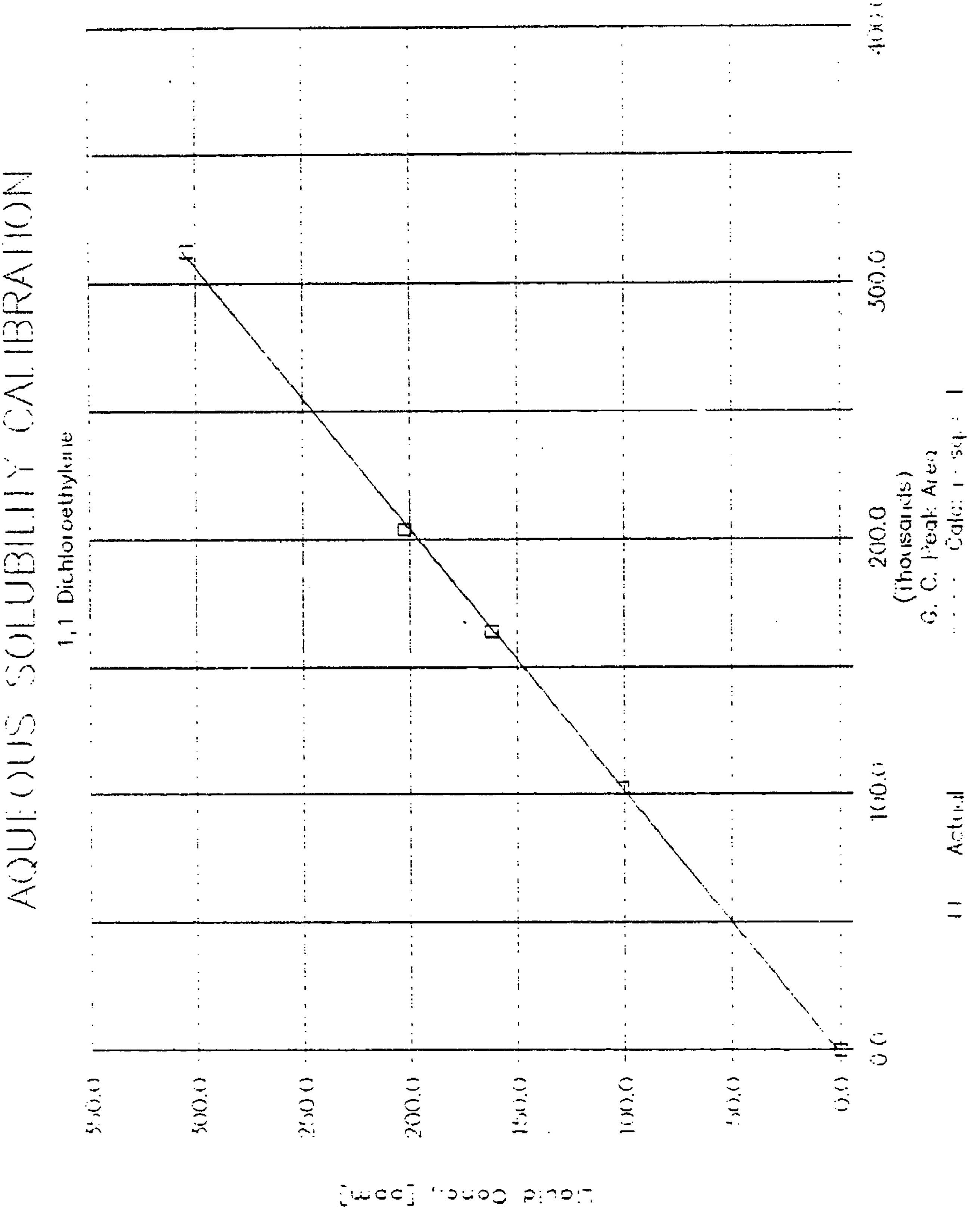

AQUEOUS SOLUBILITY CALIBRATION
Mesitylene
U.V. Detector Scale
Actual

AQUEOUS SOLUBILITY CALIBRATION

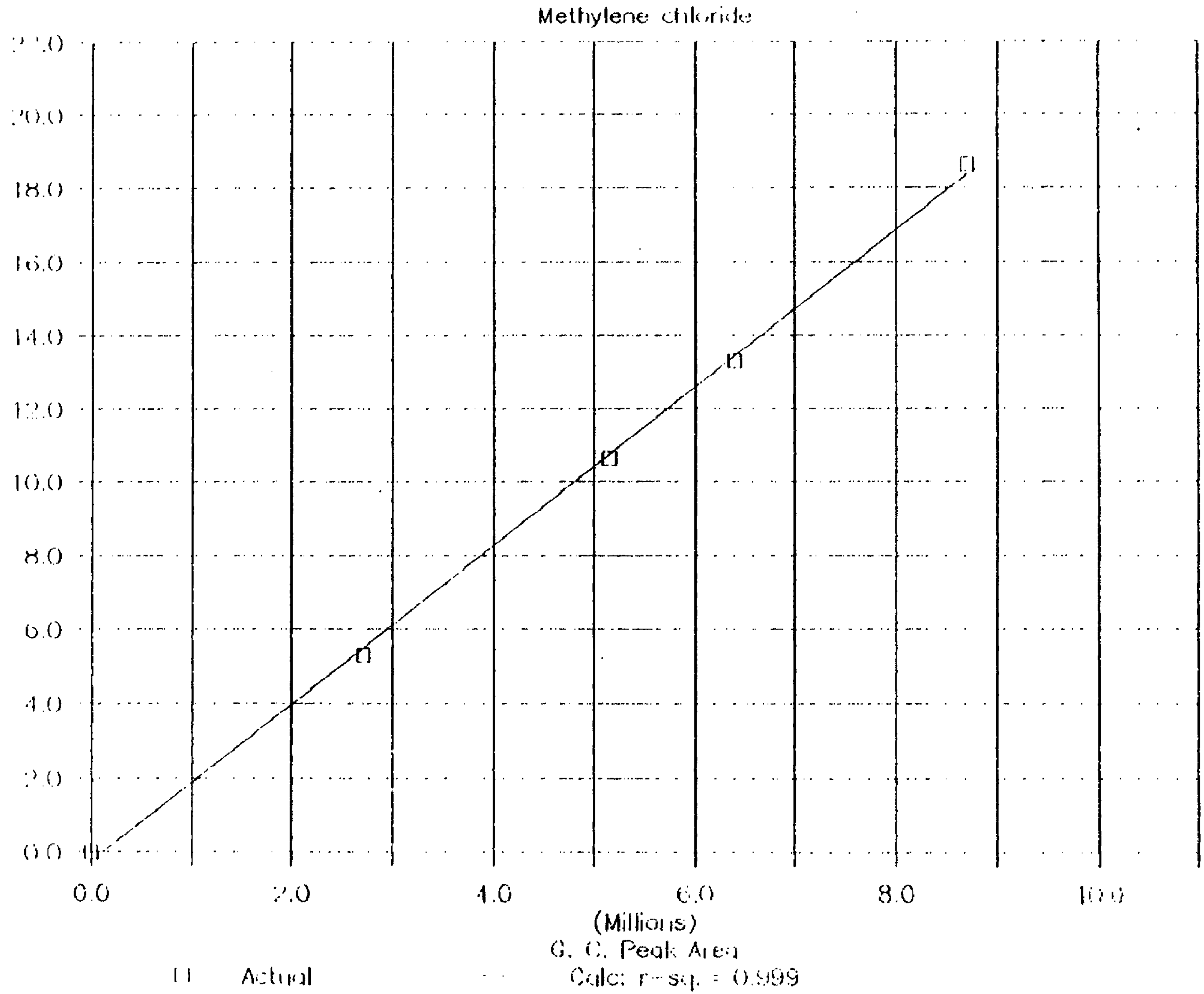



AQUEOUS SOLUBILITY CALIBRATION
Ethylene Dibromide
800.0
700.0
600.0
500.0
400.0
300.0
200.0
100.0
0.0
Liquid Conc. [ppm]
0.0
40.0
80.0
120.0
160.0
200.0
240.0
280.0
(Thousands)
G. C. Peak Area
Actual

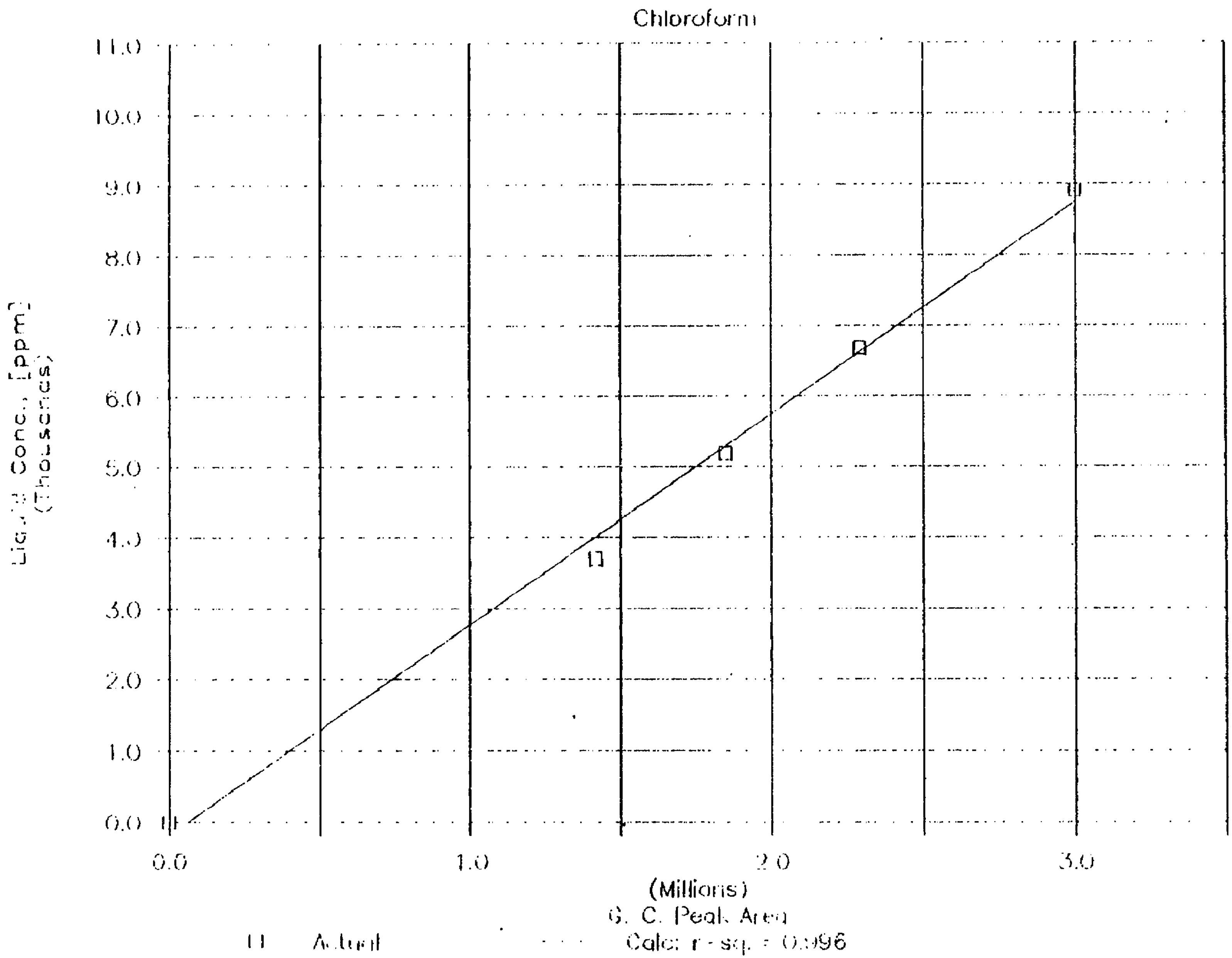

AQUEOUS SOLUBILITY CALIBRATION
1,1 Dichloroethylene
Liquid Conc. [ppm]
0.0
50.0
100.0
150.0
200.0
250.0
300.0
350.0
0.0
20.0
40.0
60.0
G. C. Peak Area
Actual

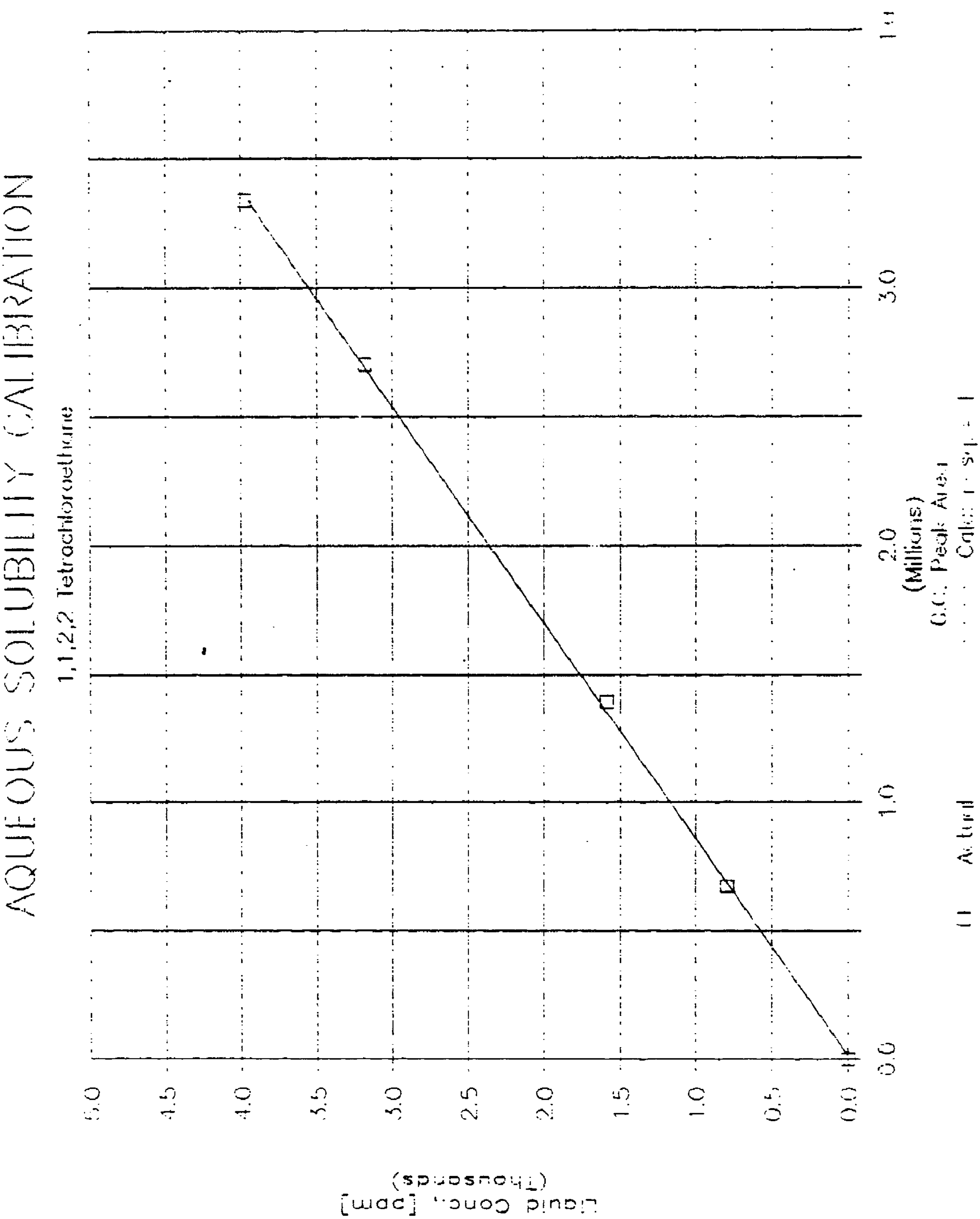

AQUEOUS SOLUBILITY CALIBRATION
1,1 Dichloroethylene
Liquid Conc. [ppm]
350.0
300.0
250.0
200.0
150.0
100.0
50.0
0.0
0.0
100.0
200.0
300.0
400.0
(Thousands)
G. C. Peak Area
Actual

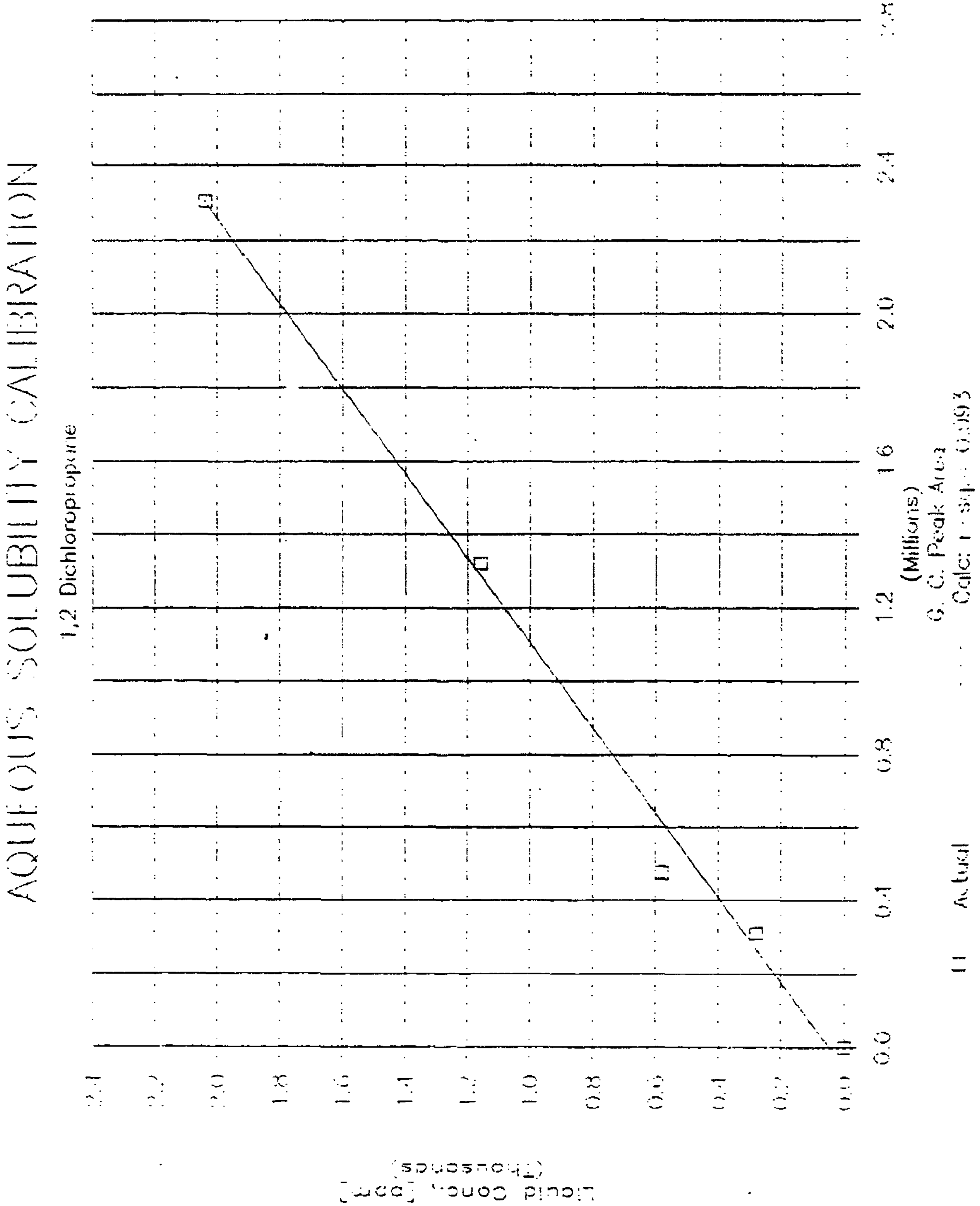
AQUEOUS SOLUBILITY CALIBRATION



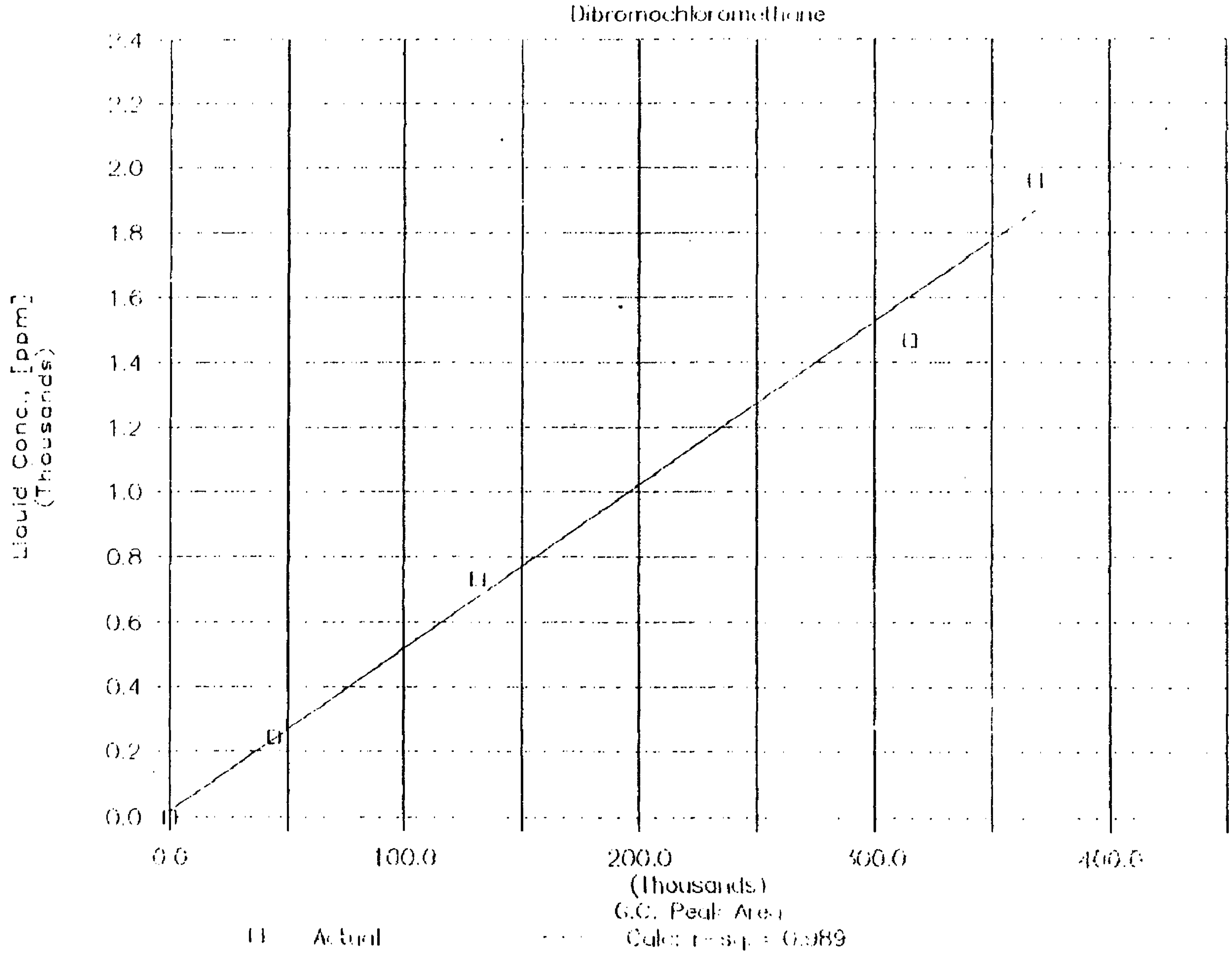
AQUEOUS SOLUBILITY CALIBRATION

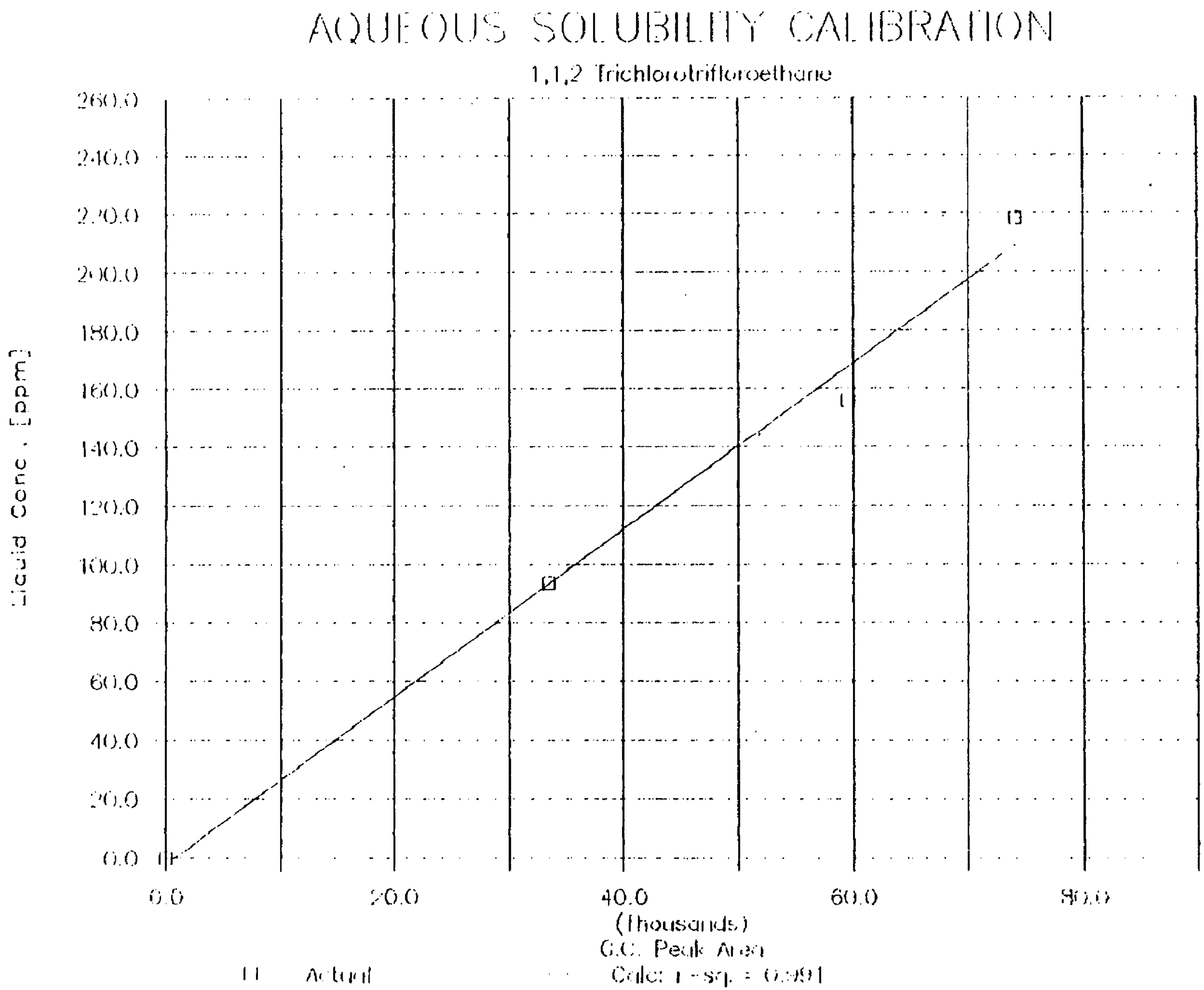


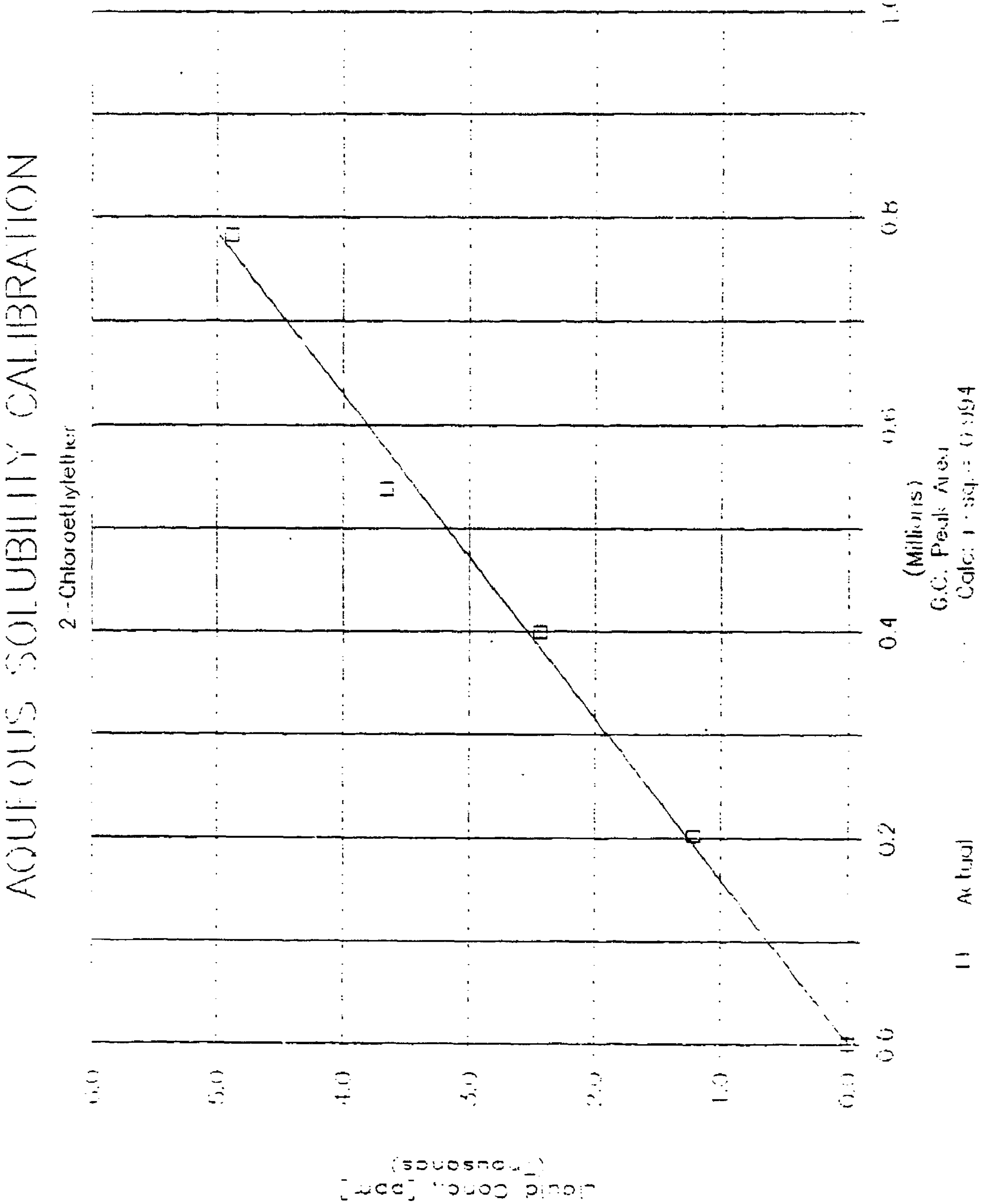

AQUEOUS SOLUBILITY CALIBRATION
1,1,2,2 Tetrachloroethane
Liquid Conc. [ppm]
(Thousands)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
0.0
1.0
2.0
3.0
(Millions)
G.C. Peak Area
Actual

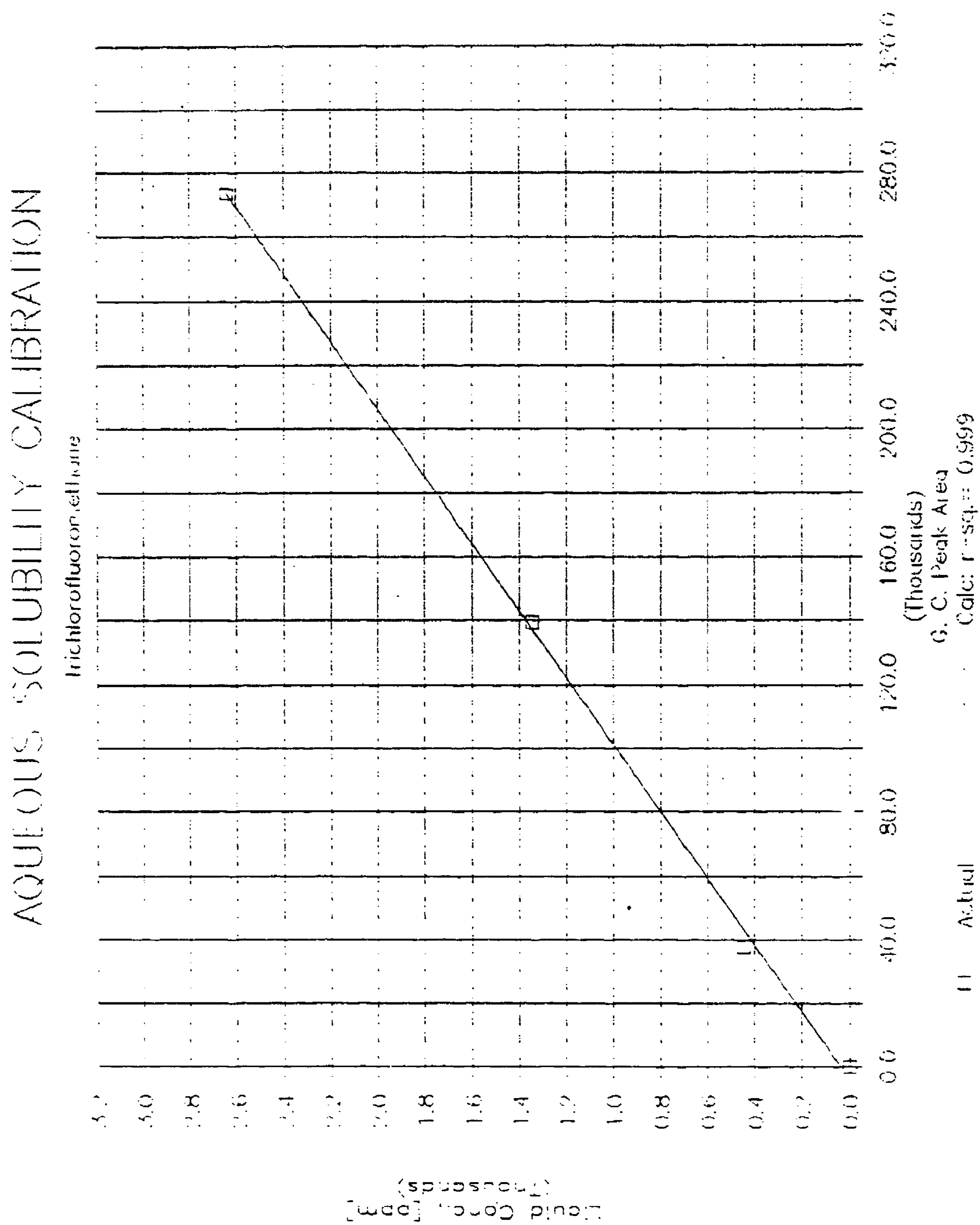

AQUEOUS SOLUBILITY CALIBRATION
1,2 Dichloropropane
0.0
0.4
0.8
1.2
1.6
2.0
2.4
(Millions)
G. C. Peak Area
Liquid Conc. [ppm]
(Thousands)
0.0
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Actual

AQUEOUS SOLUBILITY CALIBRATION




AQUEOUS SOLUBILITY CALIBRATION
1,1,2 Trichlorotrifloroethane
Liquid Conc., [ppm]
260.0
240.0
220.0
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0.0
0.0
20.0
40.0
60.0
80.0
(Thousands)
G.C. Peak Area
Actual
Calc: r-sq. = 0.991


AQUEOUS SOLUBILITY CALIBRATION
2-Chloroethylether
Liquid Conc. [ppm]
(Thousands)
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.0
0.2
0.4
0.6
0.8
1.0
(Millions)
G.C. Peak Area
Actual
Calc.



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APPENDIX D

SOFTWARE DOCUMENTATION

SOFTWARE DOCUMENTATION

This Appendix contains the Fortran source code for the simplex UNIFAC parameter fitting routine and the interactive program for calculating Henry's law constants and aqueous solubilities. The output from an example simplex fitting run is included for the interested reader. A complete Fortran listing of the UNIFAC VLE and LLE binary interaction databases is also presented in this Appendix to complete the software documentation.

EXAMPLE PARAMETER FIT WITH SIMPLEX ALGORITHM

```
**************
*            *
* CH2CO/CCOH *
*            *
**************
```

ACETONE(11)-ETHANOL(20) AT 305.15, CAN.J.RES. 24B,254,(1946)
ETHANOL(20)-2,BUTANONE(12) AT 1 ATM, ZH.PRIKL.KHIM. 41,589,(1968)
ISOPROPANOL(1)-2,PENTANONE(16) AT 1 ATM, IEC 45,1803,(1953)

COMPONENT / GROUPS

	1	2	17	15	22
11	1	0	0	0	1
20	0	0	1	0	0
12	1	1	0	0	1
16	1	2	0	0	1
1	1	0	0	1	0

GROUP NO	GROUP R	GROUP Q
1	.9011E+00	.8480E+00
2	.6744E+00	.5400E+00
17	.2106E+01	.1972E+01
15	.1878E+01	.1660E+01
22	.1672E+01	.1488E+01

GROUP INTERACTION PARAMETERS

.0000E+00	.0000E+00	.7375E+03	.7375E+03	.4764E+03
.0000E+00	.0000E+00	.7375E+03	.7375E+03	.4764E+03
-.8793E+02	-.8793E+02	.0000E+00	.0000E+00	.1000E+01
-.8793E+02	-.8793E+02	.0000E+00	.0000E+00	.1000E+01
.2676E+02	.2676E+02	.1000E+01	.1000E+01	.0000E+00

INITIAL PARAMETERS 3 5
100.000 100.000
110.000 100.000
100.000 110.000

SIMPLEX ALGORITHM RESULTS

FINAL PARAMETERS
117.240 36.630
FMIN= .54424E-01 SD= .70283E-06

TEMP	NUMBER	X	GAMEXP	GAMCAL	DEV
1					
305.15	11	.0750	2.0516	1.8340	-10.6
305.15	20	.9250	1.0055	1.0038	-.2
2					
305.15	11	.5000	1.2187	1.2088	-.8
305.15	20	.5000	1.2304	1.1903	-3.3
3					
305.15	11	.8000	1.0356	1.0330	-.3
305.15	20	.2000	1.6686	1.5984	-4.2
4					
305.15	11	1.0000	1.0000	1.0000	.0
305.15	20	.0000	2.3166	2.1507	-7.2
5					
348.15	20	.2380	1.4546	1.5372	5.7
348.15	12	.7620	1.0506	1.0463	-.4
6					
347.55	20	.3970	1.2497	1.3013	4.1
347.55	12	.6030	1.1154	1.1306	1.4
7					
347.55	20	.6220	1.0965	1.1057	.8
347.55	12	.3780	1.2825	1.3382	4.3
8					
348.45	20	.7860	1.0234	1.0321	.8
348.45	12	.2140	1.5091	1.5754	4.4
9					
350.15	20	.9340	1.0046	1.0030	-.2
350.15	12	.0660	1.7549	1.8757	6.9
10					
371.37	1	.0755	1.5221	1.5656	2.9
371.37	16	.9245	.9678	1.0028	3.6
11					
361.71	1	.3720	1.2395	1.2481	.7
361.71	16	.6280	1.0060	1.0742	6.8
12					
358.59	1	.5845	1.0974	1.1070	.9
358.59	16	.4155	1.1203	1.2018	7.3
13					
356.76	1	.7815	1.0257	1.0298	.4
356.76	16	.2185	1.2816	1.4073	9.8

```
$DEBUG
C
C
C  *********************************************************************
C  *                                                                   *
C  *      UNIFAC PARAMETER ESTIMATION BY MEANS OF                      *
C  *      NELDER-MEAD'S EXTENDED SIMPLEX MINIMIZATION METHOD           *
C  *                                                                   *
C  *********************************************************************
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(10),RS(10),QS(10),XL(10),KG(10),NTEXT(40),NUM(10),
     &IPAR(4),PAR(4),DEV(100,2),JENS(10),NU(100,2)
      DIMENSION RI(76),QI(76),AI(40,40),MAIN(76)
      DIMENSION X(5,4),F(5),XB(4),XS(4),XM(4),XE(4),XX(4),XR(4),XK(4)
      COMMON /U/ T(100),NM(100,2),XXX(100,2),GME(100,2),GMC(100,2),
     &GMR(100,2),NNY(10,10),Q(10),A(10,10)
      DATA NC,NP/5,6/
C
      OPEN(6,FILE='SIMPLEX.DAT',STATUS='OLD',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
      OPEN(7,FILE='SIMPLEX.OUT',STATUS='NEW',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
C
      READ(6,16) NCOMP,NG,NOBS,LAAF,NOIT,MDA
   16 FORMAT(20I3)
C
C         NCOMP= NUMBER OF COMPONENTS
C         NG    = NUMBER OF DIFFERENT GROUPS
C         NOBS = NUMBER OF DATA POINTS
C         LAAF,  LAAF=1 THE EXPERIMENTAL ACTIVITY COEFFICIENTS
C                       ARE READ
C                LAAF=2 THE LOGARITHMS TO THE EXPERIMENTAL
C                       ACTIVITY COEFFICIENTS ARE READ
C         NOIT,  NOIT=1 PARAMETER ESTIMATION IS PERFORMED
C                NOIT=2 NO PARAMETER ESTIMATION.  THE ACTIVITY
C                       COEFFICIENTS ARE CALCULATED BASED ON
C                       THE GIVEN R,Q AND A MATRIX
C         MDA,   MDA=1  BUILT-IN VLE PARAMETERS ARE LOADED
C                MDA=2  BUILT-IN LLE PARAMETERS ARE LOADED
C
      IF(NOIT.EQ.2) GOTO 1301
      WRITE(7,15)
      WRITE(*,15)
   15 FORMAT(1H ,'      PARAMETER ESTIMATION')
      GOTO 1302
 1301 WRITE(7,1303)
      WRITE(*,1303)
 1303 FORMAT(1H ,'      CALCULATION OF ACTIVITY COEFFICIENTS BASED ON THE
     &GIVEN R, Q, AND A MATRIX')
 1302 CONTINUE
      DO 14 I=1,16
```

```
      READ(6,13) NTEXT
      WRITE(*,13) NTEXT
   14 WRITE(7,13) NTEXT
   13 FORMAT(40A2)
      READ(6,16) (NUM(I),I=1,NCOMP)
C
C        NUM GIVES THE NUMBERS ATTACHED TO
C        THE DIFFERENT COMPONENTS
C
      DO 1304 I=1,NCOMP
 1304 READ(6,2) (NNY(I,K),K=1,NG)
    2 FORMAT(40I2)
C
C        NNY(I,K) IS THE MATRIX GIVING THE NUMBER OF GROUPS OF
C        KIND K IN MOLECULE I
C
      READ(6,16) (KG(K),K=1,NG)
C
C        KG(K) IS THE NUMBER ATTACHED TO GROUP K
C
      DO 100 N=1,NOBS
  100 READ(6,101) T(N),(NU(N,I),XXX(N,I),GME(N,I),I=1,2)
  101 FORMAT(F7.2,3(I4,2F7.4))
C
C        N          = DATA POINT NUMBER
C        T(N)       = TEMPERATURE IN K
C        NU(N,I)    = NUMBER ATTACHED TO COMPONENT I
C                     (NU(N,I)=NUM(I))
C        XXX(N,I)   = LIQUID MOLE FRACTION
C        GME(N,I),    LAAF=1 EXPERIMENTAL ACTIVITY COEFFICIENT
C                     LAAF=2 LOGARITHM TO THE EXPERIMENTAL ACTIVITY
C                            COEFFICIENT
C
      IF(LAAF-1)820,820,821
  821 CONTINUE
      DO 822 N=1,NOBS
      DO 822 I=1,2
      GGG=GME(N,I)
      GME(N,I)=DEXP(GGG)
  822 CONTINUE
  820 CONTINUE
      IF(MDA.EQ.1) CALL UVLE(RI,QI,AI,MAIN)
      IF(MDA.EQ.2) CALL ULLE(RI,QI,AI,MAIN)
      DO 705 I=1,NG
      R(I)=RI(KG(I))
      Q(I)=QI(KG(I))
      DO 705 IU=1,NG
      A(I,IU)=AI(MAIN(KG(IU)),MAIN(KG(I)))
  705 CONTINUE
      READ(6,*   ) IOWN
      IF(IOWN.EQ.0) GOTO 707
      DO 704 IU=1,IOWN
      READ(6,*   ) KOWNI
```

```
      READ(6,706) R(KOWNI),Q(KOWNI),(A(KOWNI,J),J=1,NG)
  706 FORMAT(8F10.4)
  704 CONTINUE
  707 CONTINUE
C
C         R(I) IS THE GROUP VOLUME OF GROUP I
C         Q(I) IS THE GROUP AREA OF GROUP I
C         A(I,J) IS THE GROUP INTERACTION PARAMETER
C                BETWEEN GROUPS I AND J
C         IOWN IS THE NUMBER OF SETS OF USER-SUPPLIED
C                R, Q, AND A(I,J) DATA
C         KOWNI IS THE GROUP ID NUMBER FOR A SET OF
C                USER-SUPPLIED DATA
C
      DO 7 I=1,NCOMP
      RS(I)=0.D0
      QS(I)=0.D0
      DO 8 J=1,NG
      RS(I)=RS(I)+NNY(I,J)*R(J)
      QS(I)=QS(I)+NNY(I,J)*Q(J)
    8 CONTINUE
    7 XL(I)=5.D0*(RS(I)-QS(I))-RS(I)+1.D0
      WRITE(7,5)
      WRITE(*,5)
    5 FORMAT (1H ,'   COMPONENT /   GROUPS',/)
      WRITE(7,12) (KG(I),I=1,NG)
      WRITE(*,12) (KG(I),I=1,NG)
   12 FORMAT (17X,10I3)
      DO 10 I=1,NCOMP
      WRITE(*,6) NUM(I),(NNY(I,J),J=1,NG)
   10 WRITE(7,6) NUM(I),(NNY(I,J),J=1,NG)
    6 FORMAT(10X,I3,4X,10I3)
      WRITE(7,3)
      WRITE(*,3)
    3 FORMAT(//,'  GROUP NO      GROUP R        GROUP Q',/)
      DO 11 I=1,NG
      WRITE(*,4) KG(I),R(I),Q(I)
   11 WRITE(7,4) KG(I),R(I),Q(I)
    4 FORMAT(4X,I3,5X,2E12.4)
      WRITE(7,1400)
      WRITE(*,1400)
 1400 FORMAT(//,'  GROUP INTERACTION PARAMETERS',/)
      DO 1401 I=1,NG
      WRITE(*,1402) (A(I,J),J=1,NG)
 1401 WRITE(7,1402) (A(I,J),J=1,NG)
 1402 FORMAT(10E12.4)
      DO 102 N=1,NOBS
      DO 102 I=1,2
      DO 104 J=1,NCOMP
      IF(NU(N,I)-NUM(J))104,103,104
  103 NM(N,I)=J
      GOTO 102
  104 CONTINUE
```

```
  102 CONTINUE
      CALL PFAC3(RS,QS,XL,NOBS)
      IF(NOIT-1)830,830,831
  831 CONTINUE
      CALL PFAC4(NG,NOBS)
      DO 832 NR=1,NOBS
      DO 832 I=1,2
      GMR(NR,I)=GMC(NR,I)+GMR(NR,I)
      GMR(NR,I)=DEXP(GMR(NR,I))
  832 CONTINUE
      GOTO 833
  830 CONTINUE
      READ(6,16) NPAR,KRIT,IDEN
C
C        NPAR IS THE NUMBER OF PARAMETERS TO
C        BE ESTIMATED
C
C        KRIT DETERMINES THE OBJECTIVE FUNCTION
C        IF KRIT=1, THE SUM OF THE SQUARED DIFFERENCES BETWEEN
C        THE EXPERIMENTAL AND CALCULATED ACTIVITY COEFFICIENTS
C        IS MINIMIZED
C        IF KRIT=2, THE LOGARITHMS OF THE ACTIVITY COEFFICIENTS
C        ARE USED
C
C        IDEN IS THE NUMBER OF IDENTICAL PAIRS
C        OF INTERACTION PARAMETERS
C
      READ(6,16) (IPAR(I),I=1,NPAR)
C
C        IPAR IS THE VECTOR INDICATING THE
C        PARAMETERS TO BE ESTIMATED IN THE
C        A MATRIX
C
      IF(IDEN)950,950,951
  951 IDEN=2*IDEN
      READ(6,16) (JENS(J),J=1,IDEN)
  950 CONTINUE
C
C        JENS IS THE VECTOR INDICATING THE IDENTICAL
C        PAIRS OF PARAMETERS
C
      NN=NPAR+1
      N=NPAR
      READ(6,400) (X(1,I),I=1,NPAR)
C
C        X(1,I)= ROW OF INITIAL PARAMETERS
C        NO INITIAL PARAMETER MUST BE ZERO
C
      SA=1.D-6
C
C        SA IS THE STANDARD ERROR AS DEFINED BY
C        NELDER-MEAD
C
```

```
      DO 201 J=2,NN
      DO 201 I=1,N
      IF(J-I-1)202,203,202
  203 X(J,I)=1.1DO*X(1,I)
      GOTO 201
  202 X(J,I)=X(1,I)
  201 CONTINUE
      WRITE(7,300) (IPAR(I),I=1,N)
      WRITE(*,300) (IPAR(I),I=1,N)
  300 FORMAT(//,'   INITIAL PARAMETERS',4I3/)
      DO 204 J=1,NN
      WRITE(*,400) (X(J,I),I=1,N)
  204 WRITE(7,400) (X(J,I),I=1,N)
      DO 1 J=1,NN
      DO 21 I=1,N
   21 XX(I)=X(J,I)
      CALL FMIN(NPAR,IPAR,PAR,NOBS,NG,XX,FF,KRIT,JENS,IDEN)
    1 F(J)=FF
      NF=NN
C
C        NF IS THE NUMBER OF CALCULATIONS OF F
C
      ALFA=1.DO
      BETA=0.5DO
      GAMMA=2.DO
      ITER=0
      JPR*O
  400 FORMAT(8F10.3)
C
C        ESTIMATION OF THE LOWEST VALUE OF F=FB
C
   25 FB=F(1)
      DC 98 I=1,N
   98 XB(I)=X(1,I)
      JB=1
      DO 31 J=2,NN
      IF(FB-F(J))31,31,108
  108 FB=F(J)
      JB=J
      DO 41 I=1,N
   41 XB(I)=X(J,I)
   31 CONTINUE
C
C        ESTIMATION OF THE HIGHEST VALUE OF F=FS
C
      FS=F(1)
      DO 51 I=1,N
   51 XS(I)=X(1,I)
      JS=1
      DO 61 J=2,NN
      IF(FS-F(J))111,61,61
  111 FS=F(J)
      JS=J
```

```
      DO 71 I=1,N
   71 XS(I)=X(J,I)
   61 CONTINUE
C
C        CALCULATION OF THE CENTROID XM(I) OF POINTS
C        EXCLUDING XS(I)
C
      DO 81 I=1,N
   81 XM(I)=-XS(I)
      DO 9 J=1,NN
      DO 122 I=1,N
  122 XM(I)=XM(I)+X(J,I)
    9 CONTINUE
      DO 121 I=1,N
  121 XM(I)=XM(I)/DBLE(N)
C
C        REFLECTION
C
      DO 131 I=1,N
  131 XR(I)=XM(I)+ALFA*(XM(I)-XS(I))
      CALL FMIN(NPAR,IPAR,PAR,NOBS,NG,XR,FR,KRIT,JENS,IDEN)
      NF=NF+1
C
C        EXPANSION
C
      IF(FR-FB)141,151,151
  141 DO 161 I=1,N
  161 XE(I)=XM(I)+GAMMA*(XR(I)-XM(I))
      CALL FMIN(NPAR,IPAR,PAR,NOBS,NG,XE,FE,KRIT,JENS,IDEN)
      NF=NF+1
      IF(FE-FB)17,18,18
   17 DO 19 I=1,N
      X(JS,I)=XE(I)
   19 XS(I)=XE(I)
      F(JS)=FE
C
C        CALCULATION OF THE HALTING CRITERION
C
   27 FM=0.D0
      DO 20 J=1,NN
   20 FM=FM+F(J)
      FM=FM/DBLE(NN)
      FRMS=0.D0
      DO 22 J=1,NN
   22 FRMS=(F(J)-FM)**2+FRMS
      RMS=DSQRT(FRMS/DBLE(N))
      ITER=ITER+1
      JPR=JPR+1
      IF(ITER-200)500,500,23
  500 CONTINUE
      IF(JPR-1)902,902,903
  903 CONTINUE
      IF(JPR-6)901,904,904
```

```
  904 JPR=1
  902 CONTINUE
      WRITE(7,107) ITER,NF
      WRITE(*,107) ITER,NF
  107 FORMAT(//,'   ITERATION',I4,'    NUMBER OF CALLS FOR THE SUBROUTIN
     &E',I5)
      WRITE(7,109)
      WRITE(*,109)
  109 FORMAT('      PARAMETERS')
      WRITE(7,400) (X(JS,I),I=1,N)
      WRITE(*,400) (X(JS,I),I=1,N)
      WRITE(7,106) F(JS),RMS
      WRITE(*,106) F(JS),RMS
  106 FORMAT(1H ,'  FMIN=',E14.5,'    SD=',E14.5)
  901 CONTINUE
      IF(RMS-SA)23,23,25
C
C        NEW SIMPLEX
C        FE GREATER THAN FB
C
   18 DO 26 I=1,N
      X(JS,I)=XR(I)
   26 XS(I)=XR(I)
      F(JS)=FR
      FS=FR
      GOTO 27
C
C        NEW SIMPLEX
C        FR GREATER THAN FB
C
  151 DO 30 J=1,NN
      IF(J-JS)28,30,28
   28 IF(FR-F(J))18,18,30
   30 CONTINUE
      IF(FR-FS)91,91,32
   91 DO 33 I=1,N
      X(JS,I)=XR(I)
   33 XS(I)=XR(I)
      F(JS)=FR
      FS=FR
   32 DO 34 I=1,N
   34 XK(I)=XM(I)+BETA*(XS(I)-XM(I))
      CALL FMIN(NPAR,IPAR,PAR,NOBS,NG,XK,FK,KRIT,JENS,IDEN)
      NF=NF+1
C
C        NEW SIMPLEX
C        AFTER CONTRACTION
C
      IF(FK-FS)35,35,36
   35 DO 37 I=1,N
      X(JS,I)=XK(I)
   37 XS(I)=XK(I)
      F(JS)=FK
```

```
      FS=FK
      GOTO 27
   36 DO 38 J=1,NN
      DO 39 I=1,N
   39 X(J,I)=(X(J,I)+XB(I))/2.DO
   38 CONTINUE
      GOTO 27
   23 WRITE(*,905)
      WRITE(7,905)
  905 FORMAT(//,'     FINAL PARAMETERS')
      WRITE(7,400) (X(JS,I),I=1,N)
      WRITE(*,400) (X(JS,I),I=1,N)
      WRITE(7,106) F(JS),RMS
      WRITE(*,106) F(JS),RMS
  833 CONTINUE
      DO 906 N=1,NOBS
      DO 906 I=1,2
      DEV(N,I)=(GMR(N,I)-GME(N,I))*100.DO/GME(N,I)
  906 CONTINUE
      WRITE(7,207)
      WRITE(*,207)
  207 FORMAT(//,'     TEMP NUMBER    X    GAMEXP      GAMCAL      DEV',/)
      DO 222 N=1,NOBS
      WRITE(7,16) N
      WRITE(*,16) N
      DO 223 I=1,2
      WRITE(*,96) T(N),NU(N,I),XXX(N,I),GME(N,I),GMR(N,I),DEV(N,I)
  223 WRITE(7,96) T(N),NU(N,I),XXX(N,I),GME(N,I),GMR(N,I),DEV(N,I)
   96 FORMAT(F8.2,I5,F8.4,2F14.4,F6.1)
  222 CONTINUE
      IF(NOIT-1)835,835,836
  835 CONTINUE
      WRITE(7,1400)
      WRITE(*,1400)
      DO 112 I=1,NG
      WRITE(*,1402) (A(I,J),J=1,NG)
  112 WRITE(7,1402) (A(I,J),J=1,NG)
      WRITE(7,996)
      WRITE(*,996)
  996 FORMAT(//,'     THE SUM OF THE SQUARED DIFFERENCES BETWEEN THE')
      IF(KRIT-1)997,997,998
  998 WRITE(*,995)
      WRITE(7,995)
  995 FORMAT('      LOGARITHMS TO THE')
  997 WRITE(*,999)
      WRITE(7,999)
  999 FORMAT('      EXPERIMENTAL AND CALCULATED ACTIVITY COEFFICIENTS IS
     & MINIMIZED')
  836 CONTINUE
      STOP
      END
C
C
```

```
C     ********************************************************************
C     *                                                                  *
C     *     SUBROUTINE PFAC3                                             *
C     *                                                                  *
C     *                                                                  *
C     *     SUBROUTINE PFAC3 CALCULATES THE COMBINATORIAL PART           *
C     *     OF THE ACTIVITY COEFFICIENTS                                 *
C     *                                                                  *
C     ********************************************************************
C
      SUBROUTINE PFAC3(RS,QS,XL,NOBS)
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION THETA(2),PHI(2),RS(10),QS(10),XL(10)
      COMMON /U/ T(100),NM(100,2),XXX(100,2),GME(100,2),GMC(100,2),
     &GMR(100,2),NNY(10,10),Q(10),A(10,10)
      DO 3 N=1,NOBS
      SQ=0.D0
      SR=0.D0
      SXL=0.D0
      DO 2 I=1,2
      J=NM(N,I)
      SXL=SXL+XL(J)*XXX(N,I)
      SQ=SQ+QS(J)*XXX(N,I)
    2 SR=SR+RS(J)*XXX(N,I)
      DO 3 I=1,2
      J=NM(N,I)
      THETA(I)=QS(J)/SQ
      PHI(I)=RS(J)/SR
      GMC(N,I)=DLOG(PHI(I))+5.D0*QS(J)*DLOG(THETA(I)/PHI(I))+XL(J)
     &-PHI(I)*SXL
    3 CONTINUE
      RETURN
      END
C
C
C     ********************************************************************
C     *                                                                  *
C     *     SUBROUTINE PFAC4                                             *
C     *                                                                  *
C     *                                                                  *
C     *     SUBROUTINE PFAC4 CALCULATES THE RESIDUAL PART                *
C     *     OF THE ACTIVITY COEFFICIENTS                                 *
C     *                                                                  *
C     ********************************************************************
C
      SUBROUTINE PFAC4(NG,NOBS)
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION GMOL(10),ATET(10),ANYK(10),BNYK(10),GK(10,3),P(10,10)
      COMMON /U/ T(100),NM(100,2),XXX(100,2),GME(100,2),GMC(100,2),
```

```
     &GMR(100,2),NNY(10,10),Q(10),A(10,10)
C
C         CALCULATION OF THE PSI MATRIX
C
      DO 250 NR=1,NOBS
      DO 7 I=1,NG
      DO 7 J=1,NG
    7 P(I,J)=DEXP(-A(I,J)/T(NR))
C
C         CALCULATION OF GROUP MOLE FRACTIONS
C
      DO 105 II=1,3
      IF(II-2)100,100,101
  100 SNYK=0.DO
C
C         PURE COMPONENT
C
      J=NM(NR,II)
      DO 12 K=1,NG
   12 SNYK=SNYK+DBLE(NNY(J,K))
      DO 13 K=1,NG
   13 GMOL(K)=DBLE(NNY(J,K))/SNYK
      GOTO 102
  101 SNYK=0.DO
C
C         MIXTURE
C
      DO 2 I=1,2
      J=NM(NR,I)
      DO 2 K=1,NG
    2 SNYK=SNYK+DBLE(NNY(J,K))*XXX(NR,I)
      DO 3 K=1,NG
      GNYK=0.DO
      DO 4 I=1,2
      J=NM(NR,I)
    4 GNYK=GNYK+DBLE(NNY(J,K))*XXX(NR,I)
    3 GMOL(K)=GNYK/SNYK
C
C         CALCULATION OF GROUP AREA FRACTIONS
C
  102 SNYK=0.DO
      DO 5 K=1,NG
    5 SNYK=SNYK+Q(K)*GMOL(K)
      DO 6 K=1,NG
    6 ATET(K)=Q(K)*GMOL(K)/SNYK
C
C         CALCULATION OF GAMMA K
C
      DO 9 K=1,NG
      ANYK(K)=0.DO
      DO 10 M=1,NG
      SNYK=0.DO
      DO 8 N=1,NG
```

```
    8 SNYK=SNYK+ATET(N)*P(N,M)
   10 ANYK(K)=ATET(M)*P(K,M)/SNYK+ANYK(K)
      BNYK(K)=0.D0
      DO 11 M=1,NG
   11 BNYK(K)=BNYK(K)+ATET(M)*P(M,K)
      BNYK(K)=DLOG(BNYK(K))
    9 GK(K,II)=Q(K)*(1.D0-BNYK(K)-ANYK(K))
  105 CONTINUE
      DO 201 I=1,2
      J=NM(NR,I)
      SNYK=0.D0
      DO 200 K=1,NG
  200 SNYK=SNYK+DBLE(NNY(J,K))*(GK(K,3)-GK(K,I))
  201 GMR(NR,I)=SNYK
  250 CONTINUE
      RETURN
      END
C
C
C   *******************************************************************
C   *                                                                 *
C   *      SUBROUTINE FMIN                                            *
C   *                                                                 *
C   *                                                                 *
C   *      SUBROUTINE FMIN CALCULATES F (THE OBJECTIVE FUNCTION)      *
C   *      AS A FUNCTION OF A SET OF PARAMETERS                       *
C   *                                                                 *
C   *******************************************************************
C
      SUBROUTINE FMIN(NPAR,IPAR,PAR,NOBS,NG,XX,FF,KRIT,JENS,IDEN)
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION IPAR(4),PAR(4),XX(4),JENS(10)
      COMMON /U/ T(100),NM(100,2),XXX(100,2),GME(100,2),GMC(100,2),
     &GMR(100,2),NNY(10,10),Q(10),A(10,10)
      DO 2 I=1,NPAR,2
      KI=IPAR(I)
      KJ=IPAR(I+1)
      A(KI,KJ)=XX(I)
    2 A(KJ,KI)=XX(I+1)
      IF(IDEN)9,9,8
    8 KKI=JENS(1)
      KKJ=JENS(2)
      DO 7 J=3,IDEN,2
      IKI=JENS(J)
      IKJ=JENS(J+1)
      A(IKI,IKJ)=A(KKI,KKJ)
      A(IKJ,IKI)=A(KKJ,KKI)
    7 CONTINUE
    9 CONTINUE
      CALL PFAC4(NG,NOBS)
      DO 200 NR=1,NOBS
```

```
      DO 200 I=1,2
      GMR(NR,I)=GMC(NR,I)+GMR(NR,I)
      GMR(NR,I)=DEXP(GMR(NR,I))
  200 CONTINUE
      FF=0.D0
      DO 3 N=1,NOBS
      DO 3 I=1,2
      IF(KRIT-1)10,10,20
   10 FF=FF+(GMR(N,I)-GME(N,I))**2
      GOTO 3
   20 GCAL=GMR(N,I)
      GEXP=GME(N,I)
      FF=FF+(DLOG(GCAL)-DLOG(GEXP))**2
    3 CONTINUE
      RETURN
      END
C
C
C   ******************************************************************
C   *                                                                *
C   *                                                                *
C   *         UVLE CONTAINS BUILT-IN UNIFAC VLE-PARAMETERS           *
C   *                                                                *
C   *                                                                *
C   ******************************************************************
C   *                                                                *
C   ******************************************************************
      SUBROUTINE UVLE(RI,QI,AI,MAIN)
C   ******************************************************************
C
C     THE MAIN GROUPS ARE:
C      1 CH2 ....... 2 C=C ...... 3 ACH ...... 4 ACCH2 .... 5 OH .......
C      6 CH3OH ..... 7 H2O ...... 8 ACOH ...... 9 CH2CO ... 10 CHO ......
C     11 CCOO ..... 12 HCOO .... 13 CH2O .... 14 CNH2 .... 15 CNH ......
C     16 (C)3N .... 17 ACNH2 ... 18 PYRIDINE  19 CCN ..... 20 COOH .....
C     21 CCL ...... 22 CCL2 .... 23 CCL3 .... 24 CCL4 .... 25 ACCL .....
C     26 CNO2 ..... 27 ACNO2 ... 28 CS2 ..... 29 CH3SH ... 30 FURFURAL .
C     31 DOH ...... 32 I ....... 33 BR ...... 34 C=-C .... 35 DMSO .....
C     36 ACRY ..... 37 CLCC .... 38 ACF ..... 39 DMF ..... 40 CF2 ......
C
C
C     THE SUB GROUPS ARE:
C      1 CH3 ....... 2 CH2 ...... 3 CH ....... 4 C ........ 5 CH2=CH ...
C      6 CH=CH ..... 7 CH2=C .... 8 CH=C ..... 9 C=C ..... 10 ACH ......
C     11 AC ....... 12 ACCH3 ... 13 ACCH2 ... 14 ACCH .... 15 OH .......
C     16 CH3OH .... 17 H2O ..... 18 ACOH .... 19 CH3CO ... 20 CH2CO ....
C     21 CHO ...... 22 CH3COO .. 23 CH2COO .. 24 HCOO .... 25 CH3O .....
C     26 CH2O ..... 27 CH-O .... 28 FCH2O ... 29 CH3NH2 .. 30 CH2NH2 ...
C     31 CHNH2 .... 32 CH3NH ... 33 CH2NH ... 34 CHNH .... 35 CH3N .....
C     36 CH2N ..... 37 ACNH2 ... 38 C5H5N ... 39 C5H4N ... 40 C5H3N ....
C     41 CH3CN .... 42 CH2CN ... 43 COOH .... 44 HCOOH ... 45 CH2CL ....
C     46 CHCL ..... 47 CCL ..... 48 CH2CL2 .. 49 CHCL2 ... 50 CCL2 .....
C     51 CHCL3 .... 52 CCL3 .... 53 CCL4 .... 54 ACCL .... 55 CH3NO2 ...
```

```
C     56 CH2NO2 ... 57 CHNO2 ... 58 ACNO2 ... 59 CS2 ..... 60 CH3SH ....
C     61 CH2SH .... 62 FURFURAL  63 (CH2OH)2  64 I ....... 65 BR .......
C     66 CH=-C .... 67 C=-C .... 68 DMSO .... 69 ACRY .... 70 CL(C=-C) .
C     71 ACF ...... 72 DMF-1 ... 73 DMF-2 ... 74 CF3 ..... 75 CF2 ......
C     76 CF.......
C
C************************************************************************
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AI(40,40),RR(76),QQ(76),RI(76),QI(76),MAINSG(76),
     *          MAIN(76)
      DIMENSION A1(40),A2(40),A3(40),A4(40),A5(40),A6(40),A7(40),A8(40),
     * A9(40),A10(40),A11(40),A12(40),A13(40),A14(40),A15(40),A16(40),
     *A17(40),A18(40),A19(40),A20(40),A21(40),A22(40),A23(40),A24(40),
     *A25(40),A26(40),A27(40),A28(40),A29(40),A30(40),A31(40),A32(40),
     *A33(40),A34(40),A35(40),A36(40),A37(40),A38(40),A39(40),A40(40)
      DATA MAINSG/ 4*1, 5*2, 2*3, 3*4, 1*5, 1*6, 1*7, 1*8, 2*9,1*10,
     *            2*11,1*12,4*13,3*14,3*15,2*16,1*17,3*18,2*19,2*20,
     *            3*21,3*22,2*23,1*24,1*25,3*26,1*27,1*28,2*29,1*30,
     *            1*31,1*32,1*33,2*34,1*35,1*36,1*37,1*38,2*39,3*40/
      DATA RR/0.9011,0.6744,0.4469,0.2195,1.3454,1.1167,1.1173,0.8886,
     *0.6605,0.5313,0.3652,1.2663,1.0396,0.8121,1.0,1.4311,0.92,0.8952,
     *1.6724,1.4457,0.9980,1.9031,1.6764,1.2420,1.1450,0.9183,0.6908,
     *0.9183,1.5959,1.3692,1.1417,1.4337,1.2070,0.9795,1.1865,0.9597,
     *1.0600,2.9993,2.8332,2.6670,1.8701,1.6434,1.3013,1.5280,1.4654,
     *1.2380,1.0060,2.2564,2.0606,1.8016,2.8700,2.6401,3.3900,1.1562,
     *2.0086,1.7818,1.5544,1.4199,2.0570,1.8770,1.6510,3.1680,2.4088,
     *1.2640,0.9492,1.2920,1.0613,2.8266,2.3144,0.7910,0.6948,3.0856,
     *2.6322,1.4060,1.0105,0.6150/
      DATA QQ/0.848,0.540,0.228,0.000,1.176,0.867,0.988,0.676,0.485,
     *0.400,0.120,0.968,0.660,0.348,1.200,1.432,1.400,0.680,1.488,
     *1.180,0.948,1.728,1.420,1.188,1.088,0.780,0.468,1.100,1.544,
     *1.236,0.924,1.244,0.936,0.624,0.940,0.632,0.816,2.113,1.833,
     *1.553,1.724,1.416,1.224,1.532,1.264,0.952,0.724,1.988,1.684,
     *1.448,2.410,2.184,2.910,0.844,1.868,1.560,1.248,1.104,1.650,
     *1.676,1.368,2.481,2.248,0.992,0.832,1.088,0.784,2.472,2.052,
     *0.724,0.524,2.736,2.120,1.380,0.920,0.460/
      DATA  A1/      0.000,  -200.000,    61.130,    76.500,   986.500,
     *   697.200,  1318.000,  1333.000,   476.400,   677.000,
     *   232.100,   741.400,   251.500,   391.500,   255.700,
     *   206.600,  1245.000,   287.770,   597.000,   663.500,
     *    35.930,    53.760,    24.900,   104.300,   321.500,
     *   661.500,   543.000,   153.600,   184.400,   354.550,
     *  3025.000,   335.800,   479.500,   298.900,   526.500,
     *   689.000,    -0.505,   125.800,   485.300,    -2.859/
      DATA  A2/   2520.000,     0.000,   340.700,  4102.000,   693.900,
     *  1509.000,   634.000,   547.400,   524.500,  9000.000,
     *    71.230,   468.700,   289.300,   396.000,   273.600,
     *   658.800,  9000.000,  9000.000,   405.900,   730.400,
     *    99.610,   337.100,  4584.000,  5831.000,   959.700,
     *   542.100,  9000.000,    76.302,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,   523.600,  9000.000,
     *  9000.000,   237.300,  9000.000,   320.400,  9000.000/
```

```
      DATA  A3/   -11.120,   -94.780,     0.000,   167.000,   636.100,
     *  637.350,  903.800, 1329.000,    25.770,  9000.000,
     *    5.994, 9000.000,    32.140,   161.700,   122.800,
     *   90.490,  668.200,    -4.449,   212.500,   537.400,
     *  -18.810, -144.400,  -231.900,     3.000,   538.200,
     *  168.000,  194.900,    52.070,   -10.430,   -64.690,
     *  210.400,  113.300,   -13.590,  9000.000,   169.900,
     * 9000.000,   69.110,   389.300,   245.600,  9000.000/
      DATA  A4/   -69.700,  -269.700,  -146.800,     0.000,   803.200,
     *  603.250, 5695.000,   884.900,   -52.100,  9000.000,
     * 5688.000, 9000.000,   213.100,  9000.000,   -49.290,
     *   23.500,  764.700,    52.800,  6096.000,   603.800,
     * -114.100, 9000.000,   -12.140,  -141.300,  -126.900,
     * 3629.000, 4448.000,    -9.451,  9000.000,   -20.360,
     * 4975.000, 9000.000,  -171.300,  9000.000,  4284.000,
     * 9000.000, 9000.000,   101.400,  5629.000,  9000.000/
      DATA  A5/   156.400,  8694.000,    89.600,    25.820,     0.000,
     * -137.100,  353.500,  -259.700,    84.000,   441.800,
     *  101.000,  193.100,    28.060,    83.020,    42.700,
     * -323.000, -348.200,   170.000,     6.712,   199.000,
     *   75.620, -112.100,   -98.120,   143.100,   287.800,
     *   61.110,  157.100,   477.000,   147.500,  -120.500,
     * -318.900,  313.500,   133.400,  9000.000,  -202.100,
     * 9000.000,  253.900,    44.780,  -143.900,  9000.000/
      DATA  A6/    16.510,   -52.390,   -50.000,   -44.500,   249.100,
     *    0.000, -181.000,  -101.700,    23.390,   306.400,
     *  -10.720,  193.400,  -180.600,   359.300,   266.000,
     *   53.900,  335.500,   580.500,    36.230,  -289.500,
     *  -38.320, -102.500,  -139.400,   -67.800,    17.120,
     *   75.140, 9000.000,   -31.090,    37.840,  9000.000,
     * 9000.000, 9000.000,  9000.000,  9000.000,  -399.300,
     * 9000.000,  -21.220,   -48.250,  -172.400,  9000.000/
      DATA  A7/   300.000,   692.700,   362.300,   377.600,  -229.100,
     *  289.600,    0.000,   324.500,  -195.400,  -257.300,
     *   14.420, 9000.000,   540.500,    48.890,   168.000,
     *  304.000,  213.000,   459.000,   112.600,   -14.090,
     *  325.400, 37[illegible].400,   353.700,   497.500,   678.200,
     *  220.600,  395.500,   887.100,  9000.000,   188.000,
     *    0.000, 9000.000,  9000.000,  9000.000,  -139.000,
     *  160.800, 9000.000,  9000.000,   319.000,  9000.000/
      DATA  A8/   275.800,  1665.000,    25.340,   244.200,  -451.600,
     * -265.200, -601.800,     0.000,  -356.100,  9000.000,
     * -449.400, 9000.000,  9000.000,  9000.000,  9000.000,
     * 9000.000, 9000.000,  -305.500,  9000.000,  9000.000,
     * 9000.000, 9000.000,  9000.000,  1827.000,  9000.000,
     * 9000.000, 9000.000,  9000.000,  9000.000,  9000.000,
     * -687.100, 9000.000,  9000.000,  9000.000,  9000.000,
     * 9000.000, 9000.000,  9000.000,  9000.000,  9000.000/
      DATA  A9/    26.760,   -82.920,   140.100,   365.800,   164.500,
     *  108.700,  472.500,  -133.100,     0.000,   -37.360,
     * -213.700, 9000.000,     5.202,  9000.000,  9000.000,
     * 9000.000,  937.900,   165.100,   481.700,   669.400,
     * -191.700, -284.000,  -354.600,   -39.200,   174.500,
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*   137.500, 9000.000,   216.100,   -46.280,  -163.700,
*  9000.000,    53.590,   245.200,  -246.600,   -44.580,
*  9000.000,   -44.420,  9000.000,   -61.700,  9000.000/
  DATA  A10/   505.700,  9000.000,  9000.000,  9000.000,  -404.800,
*  -340.200,   232.700,  9000.000,   128.000,     0.000,
*  9000.000,  9000.000,   304.100,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
*   751.900,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000/
  DATA A11/    114.800,   269.300,    85.840,  -170.000,   245.400,
*   249.630,10000.000,   -36.720,   372.200,  9000.000,
*     0.000,   372.900,  -235.700,  9000.000,   -73.500,
*  9000.000,  9000.000,  9000.000,   494.600,   660.200,
*  9000.000,   108.900,  -209.700,    54.570,   629.000,
*  9000.000,  9000.000,   183.000,  9000.000,   202.300,
*  -101.700,   148.300,  9000.000,  9000.000,    52.080,
*  9000.000,   -23.300,  9000.000,  9000.000,  9000.000/
  DATA A12/     90.490,    91.650,  9000.000,  9000.000,   191.200,
*   155.700,  9000.000,  9000.000,  9000.000,  9000.000,
*  -261.100,     0.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  -356.300,
*  9000.000,  9000.000,  -287.200,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,     4.339,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000/
  DATA A13/     83.360,    76.440,    52.130,    65.690,   237.700,
*   339.720,  -314.700,  9000.000,    52.380,    -7.838,
*   461.300,  9000.000,     0.000,  9000.000,   141.700,
*  9000.000,  9000.000,  9000.000,  9000.000,   664.600,
*   301.100,   137.800,  -154.300,    47.670,  9000.000,
*    95.180,  9000.000,   140.900,    -8.538,  9000.000,
*   -20.110,  -149.500,  -202.300,  9000.000,   172.100,
*  9000.000,   145.600,  9000.000,   254.800,  9000.000/
  DATA A14/    -30.480,    79.400,   -44.850,  9000.000,  -164.000,
*  -481.700,  -330.400,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,     0.000,    63.720,
*   -41.110,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,   -99.810,    68.810,
*  9000.000,  9000.000,  9000.000,   -70.140,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000/
  DATA A15/     65.330,   -41.320,   -22.310,   223.000,  -150.000,
*  -500.400,  -448.200,  9000.000,  9000.000,  9000.000,
*   136.000,  9000.000,   -49.300,   108.800,     0.000,
*  -189.200,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,    71.230,  4350.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
*  9000.000,  9000.000,  9000.000,  9000.000,  9000.000/
  DATA A16/    -83.980,  -188.000,  -223.900,   109.900,    28.600,
*  -406.800,  -598.800,  9000.000,  9000.000,  9000.000,
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     * 9000.000, 9000.000, 9000.000,   38.890,  865.900,
     *    0.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,  -73.850, -352.900,   -8.283,  -86.360,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000/
      DATA A17/ 5339.000, 9000.000,  650.400,  979.800,  529.000,
     *    5.182, -339.500, 9000.000, -399.100, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,    0.000, 9000.000, -216.800, 9000.000,
     * 9000.000, 9000.000, 9000.000, 8455.000,  699.100,
     * 9000.000,  -62.730, 9000.000, 9000.000, 9000.000,
     *  125.300, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, -293.100, 9000.000/
      DATA A18/ -101.600, 9000.000,   31.870,   49.800, -132.300,
     * -378.200, -332.900, -341.600,  -51.540, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000,    0.000, -169.700, -153.700,
     * 9000.000, -351.600, -114.700, -165.100, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000/
      DATA A19/   24.820,   34.780,  -22.970, -138.400,  185.400,
     *  157.800,  242.800, 9000.000, -287.500, 9000.000,
     * -266.600, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,  617.100,  134.300,    0.000, 9000.000,
     * 9000.000, 9000.000,  -15.620,  -54.860,   52.310,
     * 9000.000, 9000.000,  230.900,   21.370, 9000.000,
     * 9000.000, 9000.000, 9000.000, -203.000, 9000.000,
     *   81.570,  -19.140, 9000.000, 9000.000, 9000.000/
      DATA A20/  315.300,  349.200,   62.320,  268.200, -151.000,
     * 1020.000,  -66.170, 9000.000, -297.800, 9000.000,
     * -256.300,  312.500, -338.500, 9000.000, 9000.000,
     * 9000.000, 9000.000, -313.500, 9000.000,    0.000,
     *   44.420, -183.400,   76.750,  212.700, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,  -90.870, 9000.000, 9000.000, 9000.000/
      DATA A21/   91.460,  -24.360,    4.680,  122.900,  562.200,
     *  529.000,  698.200, 9000.000,  286.300,  -47.510,
     * 9000.000, 9000.000,  225.400, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000,  326.400,
     *    0.000,  108.300,  249.200,   62.420,  464.400,
     * 9000.000, 9000.000,  450.100,   59.020, 9000.000,
     * 9000.000, 9000.000, -125.900, 9000.000, 9000.000,
     * 9000.000,  -58.770, 9000.000, 9000.000, 9000.000/
      DATA A22/   34.010,  -52.710,  121.300, 9000.000,  747.700,
     *  669.900,  708.700, 9000.000,  423.200, 9000.000,
     * -132.900, 9000.000, -197.700, 9000.000, 9000.000,
     * -141.400, 9000.000,  587.300, 9000.000, 1821.000,
     *  -84.530,    0.000,    0.000,   56.330, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,  177.600, 9000.000, 9000.000,  215.000,
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     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000/
      DATA A23/    36.700, -185.100,  288.500,   33.610,  742.100,
     *  649.100,  826.760, 9000.000,  552.100, 9000.000,
     *  176.500,  488.900,  -20.930, 9000.000, 9000.000,
     * -293.700, 9000.000,   18.980,   74.040, 1346.000,
     * -157.100,    0.000,    0.000,  -30.100, 9000.000,
     * 9000.000, 9000.000,  116.600, 9000.000,  -64.380,
     * 9000.000,   86.400, 9000.000, 9000.000,  363.700,
     * 9000.000,  -79.540, 9000.000, 9000.000, 9000.000/
      DATA A24/   -78.450, -293.700,   -4.700,  134.700,  856.300,
     *  860.100, 1201.000,10000.000,  372.000, 9000.000,
     *  129.500, 9000.000,  113.900,  261.100,   91.130,
     * -126.000, 1301.000,  309.200,  492.000,  689.000,
     *   11.800,   17.970,   51.900,    0.000,  475.800,
     *  490.900,  534.700,  132.200, 9000.000,  546.700,
     * 9000.000,  247.800,   41.940, 9000.000,  337.700,
     * 9000.000,  -86.850,  215.200,  498.600, 9000.000/
      DATA A25/  -141.300, -203.200, -237.700,  375.500,  246.900,
     *  661.600,  920.400, 9000.000,  128.100, 9000.000,
     * -246.300, 9000.000, 9000.000,  203.500, -108.400,
     * 1088.000,  323.300, 9000.000,  356.900, 9000.000,
     * -314.900, 9000.000, 9000.000, -255.400,    0.000,
     * -154.500, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000,  -60.700, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000/
      DATA A26/   -32.690,  -49.920,   10.380,  -97.050,  341.700,
     *  252.600,  417.900, 9000.000, -142.600, 9000.000,
     * 9000.000, 9000.000,  -94.490, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000,  -34.680,  794.400,
     *    0.000,  533.200, 9000.000, 9000.000, 9000.000,
     *  139.800,  304.300,   10.170,  -27.700, 9000.000,
     * 9000.000,   48.400, 9000.000, 9000.000, 9000.000/
      DATA A27/  5541.000, 9000.000, 1824.000, -127.800,  561.600,
     * 9000.000,  360.700, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 5250.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000,  514.600, 9000.000,
     *  -85.120,    0.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000/
      DATA A28/   -52.650,   16.620,   21.500,   40.680,  823.500,
     *  914.200, 1081.000, 9000.000,  303.700, 9000.000,
     *  243.800, 9000.000,  112.400, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000,  335.700, 9000.000,
     *  -73.090, 9000.000,  -26.060,  -60.710, 9000.000,
     * 9000.000, 9000.000,    0.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,  -47.370, 9000.000, 9000.000, 9000.000/
      DATA A29/    -7.481, 9000.000,   28.410, 9000.000,  461.600,
     *  382.800, 9000.000, 9000.000,  160.600, 9000.000,
     * 9000.000,  239.800,   63.710,  106.700, 9000.000,
     * 9000.000, 9000.000, 9000.000,  125.700, 9000.000,
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     *   -27.940,  9000.000,  9000.000,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,     0.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,    31.660,
     *  9000.000,  9000.000,  9000.000,    78.920,  9000.000/
      DATA A30/    -25.310,  9000.000,   157.300,   404.300,   521.600,
     *  9000.000,    23.460,  9000.000,   317.500,  9000.000,
     *  -146.300,  9000.000,  9000.000,  9000.000,  9000.000,
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     *  9000.000,  9000.000,    48.480,  -133.160,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,     0.000,
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     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000/
      DATA A31/    140.000,  9000.000,   221.400,   150.600,   267.600,
     *  9000.000,     0.000,   838.400,  9000.000,  9000.000,
     *   152.000,  9000.000,     9.207,  9000.000,  9000.000,
     *  9000.000,   164.400,  9000.000,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
     *   481.300,  9000.000,  9000.000,  9000.000,  9000.000,
     *     0.000,  9000.000,  9000.000,  9000.000,  -417.200,
     *  9000.000,  9000.000,  9000.000,   302.200,  9000.000/
      DATA A32/    128.000,  9000.000,    58.680,  9000.000,   501.300,
     *  9000.000,  9000.000,  9000.000,   138.000,  9000.000,
     *    21.920,  9000.000,   476.600,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
     *  9000.000,   -40.820,    21.760,    48.490,  9000.000,
     *    64.280,  9000.000,  9000.000,  9000.000,  9000.000,
     *  9000.000,     0.000,  9000.000,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000/
      DATA A33/    -31.520,  9000.000,   155.600,   291.100,   721.900,
     *  9000.000,  9000.000,  9000.000,  -142.600,  9000.000,
     *  9000.000,  9000.000,   736.400,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
     *  1169.000,  9000.000,  9000.000,   225.800,   224.000,
     *   125.300,  9000.000,  9000.000,  9000.000,  9000.000,
     *  9000.000,  9000.000,     0.000,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000/
      DATA A34/    -72.880,  -184.400,  9000.000,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,   443.600,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,   329.100,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
     *   174.400,  9000.000,  9000.000,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,     0.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,  -119.800,  9000.000/
      DATA A35/     50.490,  9000.000,    -2.504,  -143.200,   -25.870,
     *   695.000,  -240.000,  9000.000,   110.400,  9000.000,
     *    41.570,  9000.000,  -122.100,  9000.000,  9000.000,
     *  9000.000,  9000.000,  9000.000,  9000.000,  9000.000,
     *  9000.000,  -215.000,  -343.600,   -58.430,  9000.000,
     *  9000.000,  9000.000,  9000.000,    85.700,  9000.000,
     *   535.800,  9000.000,  9000.000,  9000.000,     0.000,
     *  9000.000,  9000.000,  9000.000,   -97.710,  9000.000/
      DATA A36/   -165.900,  9000.000,  9000.000,  9000.000,  9000.000,
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     * 9000.000,  386.600, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000,  -42.310, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     *    0.000, 9000.000, 9000.000, 9000.000, 9000.000/
      DATA A37/   41.900,   -3.167,  -75.670, 9000.000,  640.900,
     *  726.700, 9000.000, 9000.000,   -8.671, 9000.000,
     *  -34.140, 9000.000, -209.300, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000,  298.400, 2344.000,
     *  201.700, 9000.000,   85.320,  143.200, 9000.000,
     *  313.800, 9000.000,  167.900, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,    0.000, 9000.000, 9000.000, 9000.000/
      DATA A38/   -5.132, 9000.000, -237.200, -157.300,  649.700,
     *  645.900, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, -124.600, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000,    0.000, 9000.000, 9000.000/
      DATA A39/  -31.950,   37.700, -133.900, -240.200,   64.160,
     *  172.200, -287.100, 9000.000,   97.040, 9000.000,
     * 9000.000, 9000.000, -158.200, 9000.000, 9000.000,
     * 9000.000,  335.600, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, -186.700, 9000.000,
     * 9000.000, 9000.000, 9000.000,  -71.000, 9000.000,
     * -191.700, 9000.000, 9000.000,    6.699,  136.600,
     * 9000.000, 9000.000, 9000.000,    0.000, 9000.000/
      DATA A40/  147.300, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000,    0.000/
      DO 5 I=1,40
      AI(I,1)=A1(I)
      AI(I,2)=A2(I)
      AI(I,3)=A3(I)
      AI(I,4)=A4(I)
      AI(I,5)=A5(I)
      AI(I,6)=A6(I)
      AI(I,7)=A7(I)
      AI(I,8)=A8(I)
      AI(I,9)=A9(I)
      AI(I,10)=A10(I)
      AI(I,11)=A11(I)
      AI(I,12)=A12(I)
      AI(I,13)=A13(I)
```

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      AI(I,14)=A14(I)
      AI(I,15)=A15(I)
      AI(I,16)=A16(I)
      AI(I,17)=A17(I)
      AI(I,18)=A18(I)
      AI(I,19)=A19(I)
      AI(I,20)=A20(I)
      AI(I,21)=A21(I)
      AI(I,22)=A22(I)
      AI(I,23)=A23(I)
      AI(I,24)=A24(I)
      AI(I,25)=A25(I)
      AI(I,26)=A26(I)
      AI(I,27)=A27(I)
      AI(I,28)=A28(I)
      AI(I,29)=A29(I)
      AI(I,30)=A30(I)
      AI(I,31)=A31(I)
      AI(I,32)=A32(I)
      AI(I,33)=A33(I)
      AI(I,34)=A34(I)
      AI(I,35)=A35(I)
      AI(I,36)=A36(I)
      AI(I,37)=A37(I)
      AI(I,38)=A38(I)
      AI(I,39)=A39(I)
      AI(I,40)=A40(I)
    5 CONTINUE
      DO 10 I=1,76
      RI(I)=RR(I)
      QI(I)=QQ(I)
      MAIN(I)=MAINSG(I)
   10 CONTINUE
      RETURN
      END
C
C
C     ******************************************************************
C     *                                                                *
C     *                                                                *
C     *           ULLE CONTAINS BUILT-IN UNIFAC LLE-PARAMETERS         *
C     *                                                                *
C     *                                                                *
C     ******************************************************************
C     *                                                                *
C     ******************************************************************
      SUBROUTINE ULLE(RI,QI,AI,MAIN)
C     ******************************************************************
C
C     THE MAIN GROUPS ARE:
C      1 CH2 ....... 2 C=C ...... 3 ACH ...... 4 ACCH2 .... 5 OH .......
C      6 P1 ........ 7 P2 ....... 8 H2O ...... 9 ACOH .... 10 CH2CO ....
C     11 CHO ...... 12 FURFURAL  13 COOH .... 14 COOC .... 15 CH2O .....
```

```
C       16 CCL ......  17 CCL2 ....  18 CCL3 ....  19 CCL4 ....  20 ACCL .....
C       21 CCN ......  22 ACNH2 ...  23 CNO2 ....  24 ACNO2 ...  25 DOH ......
C       26 DEOH .....  27 PYRIDINE   28 TCE .....  29 MFA .....  30 DMFA .....
C       31 TMS ......  32 DMSO ....
C
C
C       THE SUB GROUPS ARE:
C        1 CH3 .......  2 CH2 ......  3 CH .......  4 C ........  5 CH2=CH ...
C        6 CH=CH .....  7 CH=C .....  8 CH2=C ....  9 ACH .....  10 AC .......
C       11 ACCH3 ....  12 ACCH2 ...  13 ACCH ....  14 OH ......  15 P1 .......
C       16 P2 .......  17 H2O .....  18 ACOH ....  19 CH3CO ...  20 CH2CO ....
C       21 CHO ......  22 FURFURAL   23 COOH ....  24 HCOOH ...  25 CH3COO ...
C       26 CH2COO ...  27 CH3O ....  28 CH2O ....  29 CH-O ....  30 FCH2O ....
C       31 CH2CL ....  32 CHCL ....  33 CCL .....  34 CH2CL2 ..  35 CHCL2 ....
C       36 CCL2 .....  37 CHCL3 ...  38 CCL3 ....  39 CCL4 ....  40 ACCL .....
C       41 CH3CN ....  42 CH2CN ...  43 ACNH2 ...  44 CH3NO2 ..  45 CH2NO2 ...
C       46 CHNO2 ....  47 ACNO2 ...  48 (CH2OH)2   49 (HOMM)2O   50 C5H5N ....
C       51 C5H4N ....  52 C5H3N ...  53 CCL2=CHCL 54 HCONHCH3   55 HCON(CH3)2
C       56 (CH2)4SO2   57 (CH2)2SO
C
C**************************************************************************
C
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION AI(40,40),RR(57),QQ(57),RI(76),QI(76),MAINSG(57),
       *          MAIN(76)
        DIMENSION A1(32),A2(32),A3(32),A4(32),A5(32),A6(32),A7(32),A8(32),
       * A9(32),A10(32),A11(32),A12(32),A13(32),A14(32),A15(32),A16(32),
       *A17(32),A18(32),A19(32),A20(32),A21(32),A22(32),A23(32),A24(32),
       *A25(32),A26(32),A27(32),A28(32),A29(32),A30(32),A31(32),A32(32)
        DATA MAINSG/ 4*1, 4*2, 2*3, 3*4, 1*5, 1*6, 1*7, 1*8, 1*9,2*10,
       *            1*11,1*12,2*13,2*14,4*15,3*16,3*17,2*18,1*19,1*20,
       *            2*21,1*22,3*23,1*24,1*25,1*26,3*27,1*28,1*29,1*30,
       *            1*31,1*32/
        DATA RR/0.9011,0.6744,0.4469,0.2195,1.3454,1.1167,0.8886,1.1173,
       *0.5313,0.3652,1.2663,1.0396,0.8121,1.0000,3.2499,3.2491,0.9200,
       *0.8952,1.6724,1.4457,0.9980,3.1680,1.3013,1.5280,1.9031,1.6764,
       *1.1450,0.9183,0.6908,0.9183,1.4654,1.2380,1.0060,2.2564,2.0606,
       *1.8016,2.8700,2.6401,3.3900,1.1562,1.8701,1.6434,1.0600,2.0086,
       *1.7818,1.5544,1.4199,2.4088,4.0013,2.9993,2.8332,2.6670,3.3092,
       *2.4317,3.0856,4.0358,2.8266/
        DATA QQ/0.848,0.540,0.228,0.000,1.176,0.867,0.676,0.988,0.400,
       *0.120,0.968,0.660,0.348,1.200,3.128,3.124,1.400,0.680,1.488,
       *1.180,0.948,2.484,1.224,1.532,1.728,1.420,1.088,0.780,0.468,
       *1.100,1.264,0.952,0.724,1.988,1.684,1.448,2.410,2.184,2.910,
       *0.844,1.724,1.416,0.816,1.868,1.560,1.248,1.104,2.248,3.568,
       *2.113,1.833,1.553,2.860,2.192,2.736,3.200,2.472/
        DATA  A1/      0.000,    74.540,  -114.800,  -115.700,   644.600,
       *   329.600,   310.700,  1300.000,  2255.000,   472.600,
       *   158.100,   383.000,   139.400,   972.400,   662.100,
       *    42.140,  -243.900,     7.500,    -5.550,   924.800,
       *   696.800,   902.200,   556.700,   575.700,   527.500,
       *   269.200,  -300.000,   -63.600,   928.300,   331.000,
       *   561.400,   956.500/
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      DATA  A2/   292.300,     0.000,   340.700,  4102.000,   724.400,
     * 1731.000, 1731.000,   896.000,  9000.000,   343.700,
     * -214.700, 9000.000,  1647.000,  -577.500,   289.300,
     *   99.610,  337.100,  4583.000,  5831.000,  9000.000,
     *  405.900, 9000.000,   425.700,  9000.000,  9000.000,
     * 9000.000, 9000.000,  9000.000,   500.700,   115.400,
     *  784.400,  265.400/
      DATA  A3/   156.500,   -94.780,     0.000,   167.000,   703.900,
     *  511.500,  577.300,   859.400,  1649.000,   593.700,
     *  362.300,   31.140,   461.800,     6.000,    32.140,
     *  -18.810, 9000.000,  -231.900,  3000.000,  -878.100,
     *   29.130,    1.640,    -1.770,   -11.190,   358.900,
     *  363.500, -578.200,  9000.000,   364.200,   -58.100,
     *   21.970,   84.160/
      DATA  A4/   104.400,  -269.700,  -146.800,     0.000,  4000.000,
     *  136.600,  906.800,  5695.000,   292.600,   916.700,
     * 1218.000,  715.600,   339.100,  5688.000,   213.100,
     * -114.100, 9000.000,   -12.140,  -141.300,  -107.300,
     * 1208.000,  689.600,  3629.000,  -175.600,   337.700,
     * 1023.000, -390.700,  9000.000,  9000.000,  9000.000,
     *  238.000,  132.200/
      DATA  A5/   328.200,   470.700,    -9.210,     1.270,     0.000,
     *  937.300,  991.300,    28.730,  -195.500,    67.070,
     * 1409.000, -140.300,  -104.000,   195.600,   262.500,
     *   62.050,  272.200,   -61.570,   -41.750,  -597.100,
     * -189.300, -348.200,   -30.700,  -159.000,   536.600,
     *   53.370,  183.300,   -44.440,  9000.000,  9000.000,
     * 9000.000, 9000.000/
      DATA  A6/  -136.700,  -135.700,  -223.000,  -162.600,  -281.100,
     *    0.000,    0.000,   -61.290,  -153.200,   -47.410,
     * -344.100,  299.300,   244.400,    19.570,  1970.000,
     * -166.400,  128.600,  1544.000,   224.600,  9000.000,
     * 9000.000, 9000.000,   150.800,  9000.000,  9000.000,
     * 9000.000, 9000.000,  9000.000,  9000.000,  9000.000,
     * 9000.000, 9000.000/
      DATA  A7/  -131.900,  -135.700,  -252.000,  -273.600,  -268.800,
     *    0.000,    0.000,     5.890,  -153.200,   353.800,
     * -338.600, -241.800,   -57.980,   487.100,  1970.000,
     * -166.400,  507.800,  1544.000,  -207.000,  9000.000,
     * 9000.000, 9000.000,   150.800,  9000.000,  9000.000,
     * 9000.000, 9000.000,  9000.000,  9000.000,  9000.000,
     * 9000.000, 9000.000/
      DATA  A8/   342.400,   220.600,   372.800,   203.700,  -122.400,
     *  247.000,  104.900,     0.000,   344.500,  -171.800,
     * -349.900,   66.950,  -465.700,    -6.320,    64.420,
     *  315.900,  370.700,   356.800,   502.900,   -97.270,
     *  198.300, -109.800,  1539.000,    32.920,  -269.200,
     * 9000.000, -873.600,  1429.000,  -364.200,  -117.400,
     *   18.410, 9000.000/
      DATA  A9/  -159.800,  9000.000,  -473.200,  -470.400,   -63.150,
     * -547.200, -547.200,  -595.900,     0.000,  -825.700,
     * 9000.000, 9000.000,  9000.000,  -898.300,  9000.000,
     * 9000.000, 9000.000,  9000.000,  4894.000,  9000.000,
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     * 9000.000, -851.600, 9000.000,  -16.130, -538.600,
     * 9000.000, -637.300, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A10/   66.560,  306.100,  -78.310,  -73.870,  216.000,
     *  401.700, -127.600,  634.800, -568.000,    0.000,
     *  -37.360,  120.300, 1247.000,  258.700,    5.202,
     * 1000.000, -301.000,   12.010,  -10.880,  902.600,
     *  430.600, 1010.000,  400.000, -328.600,  211.600,
     * 9000.000, 9000.000,  148.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A11/  146.100,  517.000,  -75.300,  223.200, -431.300,
     *  643.400,  231.400,  623.700, 9000.000,  128.000,
     *    0.000, 1724.000,    0.750, -245.800, 9000.000,
     *  751.800, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A12/   14.780, 9000.000,  -10.440, -184.900,  444.700,
     *  -94.640,  732.300,  211.600, 9000.000,   48.930,
     * -311.600,    0.000, 1919.000,   57.700, 9000.000,
     * 9000.000, -347.900, -249.300,   61.590, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, -278.200,
     * 9000.000, -208.400,  -13.910, 9000.000,  173.800,
     * 9000.000, 9000.000/
      DATA A13/ 1744.000,  -48.520,   75.490,  147.300,  118.400,
     *  728.700,  349.100,  652.300, 9000.000, -101.300,
     * 1051.000, -115.700,    0.000, -117.600,  -96.620,
     *   19.770, 1670.000,   48.150,   43.830,  874.300,
     * 9000.000,  942.200,  446.300, 9000.000,  572.700,
     * 9000.000, 9000.000,   -2.160, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A14/ -320.100,  485.600,  114.800, -170.000,  180.600,
     *  -76.640, -152.800,  385.900, -337.300,   58.840,
     * 1090.000,  -46.130, 1417.000,    0.000, -235.700,
     * 9000.000,  108.900, -209.700,   54.570,  629.000,
     * -149.200, 9000.000, 9000.000, 9000.000,  343.100,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A15/ 1571.000,   76.440,   52.130,   65.690,  137.100,
     * -218.100, -218.100,  212.800, 9000.000,   52.380,
     * 9000.000, 9000.000, 1402.000,  461.300,    0.000,
     *  301.100,  137.800, -154.300,   47.670, 9000.000,
     * 9000.000, 9000.000,   95.180, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A16/   73.800,  -24.360,    4.680,  122.900,  455.100,
     *  351.500,  351.500,  770.000, 9000.000,  483.900,
     *  -47.510, 9000.000,  337.100, 9000.000,  225.400,
     *    0.000,  110.500,  249.200,   62.420, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A17/   27.900,  -52.710, 9000.000, 9000.000,  669.200,
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     * -186.100, -401.600,  740.400, 9000.000,  550.600,
     * 9000.000,  808.800,  437.700, -132.900, -197.700,
     *  -21.350,    0.000, 9000.000,   56.330, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A18/   21.230, -185.100,  288.500,   33.610,  418.400,
     * -465.700, -465.700,  793.200, 9000.000,  342.200,
     * 9000.000,  203.100,  370.400,  176.500,  -20.930,
     * -157.100, 9000.000,    0.000,  -30.100, 9000.000,
     *   70.040,  -75.500, 9000.000, 9000.000, 9000.000,
     * 9000.000,   18.980, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A19/   89.970, -293.700,   -4.700,  134.700,  713.500,
     * -260.300,  512.200, 1205.000, 1616.000,  550.000,
     * 9000.000,   70.140,  438.100,  129.500,  113.900,
     *   11.800,   17.970,   51.900,    0.000,  475.800,
     *  492.000, 1302.000,  490.900,  534.700, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A20/  -59.060, 9000.000,  777.800,  -47.130, 1989.000,
     * 9000.000, 9000.000,  390.700, 9000.000,  190.500,
     * 9000.000, 9000.000, 1349.000, -246.300, 9000.000,
     * 9000.000, 9000.000, 9000.000, -255.400,    0.000,
     *  346.200, 9000.000, -154.500, 9000.000,  124.800,
     * 9000.000, -387.700, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A21/   29.080,   34.780,   56.410,  -53.290, 2011.000,
     * 9000.000, 9000.000,   63.480, 9000.000, -349.200,
     * 9000.000, 9000.000, 9000.000,    2.410, 9000.000,
     * 9000.000, 9000.000,  -15.620,  -54.860, -465.200,
     *    0.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,  134.300, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A22/  175.800, 9000.000, -218.900,  -15.410,  529.000,
     * 9000.000, 9000.000, -239.800, -860.300,  857.700,
     * 9000.000, 9000.000,  681.400, 9000.000, 9000.000,
     * 9000.000, 9000.000, -216.300, 8455.000, 9000.000,
     * 9000.000,    0.000, 9000.000,  179.900,  125.300,
     * 9000.000,  924.500, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A23/   94.340,  375.400,  113.600,  -97.050,  483.800,
     *  264.700,  264.700,   13.320, 9000.000,  377.000,
     * 9000.000, 9000.000,  152.400, 9000.000,  -94.490,
     * 9000.000, 9000.000, 9000.000,  -34.680,  794.400,
     * 9000.000, 9000.000,    0.000, 9000.000,  139.800,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A24/  193.600, 9000.000,    7.180, -127.100,  332.600,
     * 9000.000, 9000.000,  439.900, -230.400,  211.600,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000,  514.600, 9000.000,
     * 9000.000,  175.800, 9000.000,    0.000,  963.000,
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     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A25/   108.500, 9000.000,  247.300,  453.400, -289.300,
     * 9000.000, 9000.000, -424.300,  523.000,   82.770,
     * 9000.000,  -75.230,-1707.000,   29.860, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, -241.700,
     * 9000.000,  164.400,  481.300, -246.000,    0.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A26/    81.490, 9000.000,  -50.710,  -30.280,  -99.560,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     *    0.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A27/  -128.800, 9000.000, -225.300, -124.600, -319.200,
     * 9000.000, 9000.000,  203.000, -222.700, 9000.000,
     * 9000.000, -201.900, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, -114.700, 9000.000, -906.500,
     * -169.700, -944.900, 9000.000, 9000.000, 9000.000,
     * 9000.000,    0.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A28/   147.300, 9000.000, 9000.000, 9000.000,  837.900,
     * 9000.000, 9000.000, 1153.000, 9000.000,  417.400,
     * 9000.000,  123.200,  639.700, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000,    9.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000,    0.000, 9000.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A29/   -11.910,  176.700,  -80.480, 9000.000, 9000.000,
     * 9000.000, 9000.000, -311.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000,    0.000, 9000.000,
     * 9000.000, 9000.000/
      DATA A30/    14.910,  132.100,  -17.780, 9000.000, 9000.000,
     * 9000.000, 9000.000, -262.600, 9000.000, 9000.000,
     * 9000.000, -281.900, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000,    0.000,
     * 9000.000, 9000.000/
      DATA A31/    67.840,   42.730,   59.160,   26.590, 9000.000,
     * 9000.000, 9000.000,    1.110, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     *    0.000, 9000.000/
      DATA A32/    36.420,   60.820,   29.770,   55.970, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
```

```
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000, 9000.000, 9000.000, 9000.000, 9000.000,
     * 9000.000,     0.000/
      DO 5 I=1,32
      AI(I,1)=A1(I)
      AI(I,2)=A2(I)
      AI(I,3)=A3(I)
      AI(I,4)=A4(I)
      AI(I,5)=A5(I)
      AI(I,6)=A6(I)
      AI(I,7)=A7(I)
      AI(I,8)=A8(I)
      AI(I,9)=A9(I)
      AI(I,10)=A10(I)
      AI(I,11)=A11(I)
      AI(I,12)=A12(I)
      AI(I,13)=A13(I)
      AI(I,14)=A14(I)
      AI(I,15)=A15(I)
      AI(I,16)=A16(I)
      AI(I,17)=A17(I)
      AI(I,18)=A18(I)
      AI(I,19)=A19(I)
      AI(I,20)=A20(I)
      AI(I,21)=A21(I)
      AI(I,22)=A22(I)
      AI(I,23)=A23(I)
      AI(I,24)=A24(I)
      AI(I,25)=A25(I)
      AI(I,26)=A26(I)
      AI(I,27)=A27(I)
      AI(I,28)=A28(I)
      AI(I,29)=A29(I)
      AI(I,30)=A30(I)
      AI(I,31)=A31(I)
      AI(I,32)=A32(I)
    5 CONTINUE
      DO 10 I=1,57
      RI(I)=RR(I)
      QI(I)=QQ(I)
      MAIN(I)=MAINSG(I)
   10 CONTINUE
      RETURN
      END
```

```
C
C  *****************************************************************
C  *
C  *          <<< MAIN PROGRAM TO CALL UNIFAC SUBROUTINES >>>
C  *
C  *
C  *     RTI INTERACTIVE VERSION: 10-8-86  (WRITTEN BY TONY ROGERS)
C  *
C  *****************************************************************
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*25 NCOMP
      DIMENSION X(10),ACT(10),DACT(10,10),TACT(10),DLACT(10),PVAP(10),
     *          AI(40,40),RI(76),QI(76),MAIN(76),NCOMP(10),HENRY(10)
      DATA MDL /3/
      DATA LIQ /0/
      DATA NVAP /1/
      DATA NC /2/
      DATA IPASS /0/
      DATA IFLAG /0/
      DATA NH /0/
C
C        --- SET UP I/O FILE NAMES ---
C
      OPEN(6,FILE='UNIFAC.DAT',STATUS='OLD',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
      OPEN(7,FILE='UNIFAC.OUT',STATUS='NEW',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
      OPEN(8,FILE='IOWN.DAT',STATUS='OLD',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
C
    1 READ(6,*) MODEL,IOUT,NDIF,NACT,LIQ
      IF(IPASS.GT.0) GOTO 2
C
      IF(IOUT.GT.0) OPEN(IOUT,FILE='BACKUP.OUT',STATUS='NEW',
     +ACCESS='SEQUENTIAL',FORM='FORMATTED')
C
C        --- PRINT "START-UP" MESSAGES ---
C
    2 IF(LIQ.GT.0) GOTO 5
      WRITE(7,901)
      WRITE(*,901)
         GOTO 10
    5 WRITE(7,902)
      WRITE(*,902)
C
C        --- INTERACTIVE READ STATEMENTS ---
C
   10 WRITE(*,'(1X,A\)') 'Enter database ID: [1] for VLE, [2] for LLE,
     &r [3] for "Environmental" ==> '
      READ(*,'(BN,I3)') MDL
      IF((MDL.NE.1).AND.(MDL.NE.2).AND.(MDL.NE.3)) GOTO 10
```

```
      WRITE(*,'(/)')
C
      IF(LIQ.GT.0) GOTO 100
C
   20 WRITE(*,'(1X,A\)') 'Enter total number of components ==> '
      READ(*,'(BN,I3)') NC
      IF((NC.LE.0).OR.(NC.GT.10)) GOTO 20
      WRITE(*,'(/)')
      IF(NC.GE.2) GOTO 30
C
C         --- ERROR MESSAGE FOR NUMBER OF COMPONENTS ---
C
      WRITE(*,'(5X,A)') '* Number of components must be 2 or greater! *'
      WRITE(*,'(//)')
      GOTO 130
C
   30 WRITE(*,'(1X,A\)') 'Enter absolute temperature in [K] ==> '
      READ(*,*) T
      IF(T.LE.0.D0) GOTO 30
      WRITE(*,'(/)')
C
      DO 35 L=1,NC
      WRITE(*,'(5X,A,I2,A\)') 'Name (<25 chars.) for Component',L,
     &' ==> '
      READ(*,'(BN,A)') NCOMP(L)
      WRITE(*,'(5X,A,I2,A\)') 'Liquid mole fraction for Component',L,
     &' ==> '
      READ(*,*) X(L)
      WRITE(*,'(/)')
   35 CONTINUE
      WRITE(*,'(/)')
C
   40 WRITE(*,'(1X,A\)') 'Calculate K-factors (y/x) for components? [1=Y
     &, 0=N] ==> '
      READ(*,'(BN,I3)') NH
      IF((NH.NE.0).AND.(NH.NE.1)) GOTO 40
      WRITE(*,'(/)')
      IF(NH.EQ.0) GOTO 100
C
   50 WRITE(*,'(1X,A\)') 'Enter [1] for vapor pressure entry, [2] for An
     &toine coefficients ==> '
      READ(*,'(BN,I3)') NVAP
      IF((NVAP.NE.1).AND.(NVAP.NE.2)) GOTO 50
      WRITE(*,'(/)')
      IF(NVAP.EQ.2) GOTO 60
C
      DO 55 K=1,NC
      WRITE(*,'(5X,A,I2,A\)') 'Enter Component',K,' v.p. in mm Hg ==> '
      READ(*,*) PVAP(K)
   55 CONTINUE
C
      WRITE(*,'(/)')
      GOTO 100
```

```
C
  60  DO 70 K=1,NC
      WRITE(*,'(5X,A,I2,A\)') 'Antoine Coefficient A (v.p. in mm Hg) for
     & Comp.',K,' ==> '
      READ(*,*) ANTA
      WRITE(*,'(5X,A,I2,A\)') 'Antoine Coefficient B (v.p. in mm Hg) for
     & Comp.',K,' ==> '
      READ(*,*) ANTB
      WRITE(*,'(5X,A,I2,A\)') 'Antoine Coefficient C (v.p. in mm Hg) for
     & Comp.',K,' ==> '
      READ(*,*) ANTC
      PVAP(K)=DEXP(ANTA-ANTB/(T+ANTC))/760.D0
      WRITE(*,'(/)')
   70 CONTINUE
C
  100 IF(MDL.EQ.1) CALL UVLE(RI,QI,AI,MAIN)
      IF(MDL.EQ.2) CALL ULLE(RI,QI,AI,MAIN)
      IF(MDL.EQ.3) CALL ENVIRON(RI,QI,AI,MAIN)
      IF(LIQ.GT.0) GOTO 120
         CALL FINOUT(NC,RI,QI,AI,MAIN,NG)
         REWIND 8
C
         WRITE(*,'(//)')
         PAUSE
         WRITE(*,'(//)')
C
         CALL PARAM(NC,NG,T)
         CALL UNIFA(NDIF,NACT,NC,NG,T,X,ACT,DACT,TACT)
C
C        --- CALCULATE K-VALUES [Y/X] FOR ALL COMPONENTS (NH=1) ---
C
         WRITE(7,903) T
         WRITE(*,903) T
      DO 110 K=1,NC
         HENRY(K)=-999.D0
         IF(NH.GT.0) HENRY(K)=ACT(K)*PVAP(K)
         WRITE(7,904) K,NCOMP(K),X(K),ACT(K),HENRY(K)
         WRITE(*,904) K,NCOMP(K),X(K),ACT(K),HENRY(K)
         WRITE(7,905)
         WRITE(*,905)
  110 CONTINUE
C
      GOTO 130
C
C        --- CALCULATION OF AQUEOUS SOLUBILITIES (LIQ=1) ---
C
  120 CALL XLIQUID(NC,MDL,MODEL,IOUT,NDIF,NACT,RI,QI,AI,MAIN)
C
  130 CONTINUE
C
C        --- USER PROMPT TO RE-START PROGRAM OR END ---
C
      WRITE(*,'(//1X,A\)') 'Enter [1] to re-start program or [0] to end
```

```
     &==> '
      READ(*,'(BN,I3)') IFLAG
      IF((IFLAG.NE.0).AND.(IFLAG.NE.1)) GOTO 130
      WRITE(*,'(//////)')
      IF(IFLAG.EQ.0) GOTO 999
      REWIND 6
      IFLAG=0
      IPASS=1
      GOTO 1
  999 CONTINUE
C
      STOP
C
C         --- FORMAT STATEMENTS ---
C
  901 FORMAT(20X,'*** ACTIVITY COEFFICIENT CALCULATION ***',///,
     &10X,'NOTE: Vapor pressure data (or Antoine coefficients) must be s
     &upplied', /,16X,'for all components to calculate their Henry"s Con
     &stants',///)
  902 FORMAT(15X,'*** BINARY LIQUID-LIQUID EQUILIBRIUM ROUTINE ***',///,
     &10X,'NOTE: Enter the most dilute chemical as Component #1.',///)
  903 FORMAT(25X,'TEMP. =',F8.2,' [K]',//,5X,'ID #',5X,'COMPONENT NAME',
     &4X,'LIQ. M-FRAC',5X,'ACT. COEFF.',5X,'H (TU)',//)
  904 FORMAT(6X,I2,6X,A15,2X,E13.5,3X,F12.5,3X,F8.1)
  905 FORMAT(///)
      END
C
C
C  ********************************************************************
C  *                                                                  *
C  *                                                                  *
C  *      <<< SUBROUTINE TO HANDLE INPUT/OUTPUT OF DATA >>>           *
C  *                                                                  *
C  *                                                                  *
C  ********************************************************************
      SUBROUTINE FINOUT(NC,RI,QI,AI,MAIN,NG)
C  ********************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/UNIF/RT(10,10),QT(10,10),TAU(10,10),S(10,10),F(10),Q(10),
     *            R(10),P(10,10)
      DIMENSION AI(40,40),RI(76),QI(76),MAIN(76),
     *          NGM(10),MS(10,10,2),NY(10,20),JH(76),IH(20)
C
      IF(IOUT.EQ.0) IOUT=7
      NK=NC
C
      DO 10 I=1,10
      DO 10 J=1,NK
         QT(I,J)=0.D0
         RT(I,J)=0.D0
   10 CONTINUE
C
      IF(MODEL.NE.1) GO TO 30
```

```
      NG=NK
C
      DO 20 I=1,NK
         READ(8,*) PT(I,I),QT(I,I),(P(I,J),J=1,NK)
   20 CONTINUE
   30 CONTINUE
C
      IF(MODEL.EQ.1) GO TO 290
      READ(8,*) IOWNRQ,IOWNP
      IF(IOWNRQ.EQ.0) GO TO 50
C
      DO 40 I=1,IOWNRQ
         READ(8,*) K,RI(K),QI(K)
   40 CONTINUE
C
   50 IF(IOWNP.EQ.0) GO TO 70
C
      DO 60 I=1,IOWNP
         READ(8,*) J,K,AI(J,K)
   60 CONTINUE
   70 CONTINUE
C
      DO 80 I=1,NK
      DO 80 J=1,10
      DO 80 K=1,2
         MS(I,J,K)=0
   80 CONTINUE
C
      DO 90 I=1,76
         JH(I)=0
   90 CONTINUE
C
      NMAX=0
      DO 100 I=1,NK
         WRITE(*,'(1X,A,I2,A\)') 'Enter number of types of subGroups in
     &component',I,' ==> '
         READ(*,'(BN,I3)') NGRP
         WRITE(*,'(/)')
C
         DO 95 KR=1,NGRP
           WRITE(*,'(5X,A,I2,A\)') 'Enter ID# of subGroup',KR,' ==> '
           READ(*,'(BN,I3)') MS(I,KR,1)
           WRITE(*,'(5X,A,I3,A,I2,A\)') 'Enter number of subGroup',KR,
     &     ' in component',I,' ==> '
           READ(*,'(BN,I3)') MS(I,KR,2)
           WRITE(*,'(/)')
   95    CONTINUE
         WRITE(*,'(/)')
C
         IF(NGRP.GT.NMAX) NMAX=NGRP
  100 CONTINUE
C
       IC=1
```

```
C
      DO 160 I=1,NK
C
         DO 150 J=1,NMAX
            IF(MS(I,J,1).EQ.0) GO TO 160
            IH(IC)=MS(I,J,1)
            IF(IC.EQ.1) GO TO 140
            IF(IH(IC).EQ.IH(IC-1)) GO TO 150
            IF(IH(IC).GT.IH(IC-1)) GO TO 140
            IF(IC.GT.2) GO TO 110
            IHH=IH(1)
            IH(1)=IH(2)
            IH(2)=IHH
            GO TO 140
  110       I1=IC-1
C
            DO 130 I2=1,I1
               IF(IH(IC).GT.IH(I2)) GO TO 130
               IF(IH(IC).EQ.IH(I2)) GO TO 150
               I4=IC-I2
C
               DO 120 I3=1,I4
                  IH(IC+1-I3)=IH(IC-I3)
  120          CONTINUE
C
               IH(I2)=MS(I,J,1)
  130       CONTINUE
C
  140       IC=IC+1
            IF(IC.GT.20) WRITE(7,905)
            IF(IC.GT.20) WRITE(*,905)
            IF(IOUT.NE.7.AND.IC.GT.20) WRITE(IOUT,905)
  150    CONTINUE
C
  160 CONTINUE
C
      IC=IC-1
C
      DO 170 I=1,IC
         JH(IH(I))=I
  170 CONTINUE
C
      DO 180 I=1,10
      DO 180 J=1,20
         NY(I,J)=0
  180 CONTINUE
C
      DO 200 I=1,NK
C
         DO 190 J=1,10
            IF(MS(I,J,1).EQ.0) GO TO 200
            N1=MS(I,J,1)
            N2=MS(I,J,2)
```

```
            IF(N1.EQ.0) GO TO 200
            N3=JH(N1)
            NY(I,N3)=N2
  190     CONTINUE
C
  200 CONTINUE
C
      I=0
      NGMGL=0
C
      DO 210 K=1,IC
         NSG=IH(K)
         NGMNY=MAIN(NSG)
         IF(NGMNY.NE.NGMGL) I=I+1
         NGM(I)=NGMNY
         NGMGL=NGMNY
      DO 210 J=1,NK
         RT(I,J)=RT(I,J)+NY(J,K)*RI(NSG)
         QT(I,J)=QT(I,J)+NY(J,K)*QI(NSG)
  210 CONTINUE
C
      NG=I
      WRITE(7,906) (IH(K),K=1,IC)
      WRITE(*,906) (IH(K),K=1,IC)
      WRITE(7,907) (MAIN(IH(K)),K=1,IC)
      WRITE(*,907) (MAIN(IH(K)),K=1,IC)
      WRITE(7,908)
      WRITE(*,908)
C
      DO 220 I=1,NK
         WRITE(*,909) I,(NY(I,K),K=1,IC)
         WRITE(7,909) I,(NY(I,K),K=1,IC)
  220 CONTINUE
C
      WRITE(7,913)
      WRITE(*,913)
      IF(IOUT.EQ.7) GO TO 240
      WRITE(IOUT,906) (IH(K),K=1,IC)
      WRITE(IOUT,907) (MAIN(IH(K)),K=1,IC)
      WRITE(IOUT,908)
C
      DO 230 I=1,NK
         WRITE(IOUT,909) I,(NY(I,K),K=1,IC)
  230 CONTINUE
C
      WRITE(IOUT,913)
  240 CONTINUE
C
      DO 250 I=1,NG
      DO 250 J=1,NG
         NI=NGM(I)
         NJ=NGM(J)
         P(I,J)=AI(NJ,NI)
```

```
  250 CONTINUE
C
      WRITE(7,910)
      WRITE(*,910)
C
      DO 260 K=1,IC
         NN=IH(K)
         WRITE(*,911) NN,RI(NN),QI(NN)
         WRITE(7,911) NN,RI(NN),QI(NN)
  260 CONTINUE
C
      WRITE(7,913)
      WRITE(*,913)
      IF(IOUT.EQ.7) GO TO 280
      WRITE(IOUT,910)
C
      DO 270 K=1,IC
         NN=IH(K)
         WRITE(IOUT,911) NN,RI(NN),QI(NN)
  270 CONTINUE
C
      WRITE(IOUT,913)
C
  280 CONTINUE
  290 CONTINUE
C
      WRITE(7,902)
      WRITE(*,902)
C
      DO 300 I=1,NG
         WRITE(*,901) (P(I,J),J=1,NG)
         WRITE(7,901) (P(I,J),J=1,NG)
  300 CONTINUE
C
      WRITE(7,913)
      WRITE(*,913)
      IF(MODEL.EQ.0) WRITE(7,903)
      IF(MODEL.EQ.0) WRITE(*,903)
      IF(MODEL.EQ.1) WRITE(7,912)
      IF(MODEL.EQ.1) WRITE(*,912)
      IF(IOUT.EQ.7) GO TO 320
      WRITE(IOUT,902)
C
      DO 310 I=1,NG
         WRITE(IOUT,901) (P(I,J),J=1,NG)
  310 CONTINUE
C
      WRITE(IOUT,913)
      IF(MODEL.EQ.0) WRITE(IOUT,903)
      IF(MODEL.EQ.1) WRITE(IOUT,912)
  320 CONTINUE
C
      DO 330 I=1,NK
```

```
          Q(I)=0.D0
          R(I)=0.D0
       DO 330 K=1,NG
          Q(I)=Q(I)+QT(K,I)
          R(I)=R(I)+RT(K,I)
  330 CONTINUE
C
       DO 340 I=1,NK
          WRITE(*,904) I,R(I),Q(I)
          WRITE(7,904) I,R(I),Q(I)
  340 CONTINUE
C
       IF(IOUT.EQ.7) GO TO 360
C
       DO 350 I=1,NK
          WRITE(IOUT,904) I,R(I),Q(I)
  350 CONTINUE
  360 CONTINUE
C
C          --- FORMAT STATEMENTS ---
C
  901 FORMAT(1X,10F12.3)
  902 FORMAT(2X,'INTERACTION PARAMETERS',/)
  903 FORMAT(1X,'UNIFAC MOLECULAR R AND Q',/)
  904 FORMAT(I5,2F15.4)
  905 FORMAT(1X,'** WARNING: NO. OF SUBGROUPS MUST NOT EXCEED 20 **')
  906 FORMAT(/,1X,'SUB GROUPS :',20I3)
  907 FORMAT(1X,'MAIN GROUPS:',20I3)
  908 FORMAT(1X,'COMPONENT')
  909 FORMAT(6X,I2,5X,20I3)
  910 FORMAT(1X,'GROUP R- AND Q-VALUES',/)
  911 FORMAT(1X,I3,2F10.4)
  912 FORMAT(1X,'SPECIFIED UNIQUAC R AND Q',/)
  913 FORMAT(//)
      RETURN
      END
C
C
C************************************************************************
C
C             <<< UNIFAC BINARY LIQUID-LIQUID FLASH ROUTINE >>>
C
C
C      NEWTON-RAPHSON ALGORITHM (GAUSS-JORDAN MAXIMUM PIVOT STRATEGY)
C------------------------------------------------------------------------
C    THIS IS A SUBROUTINE TO IMPLEMENT THE NEWTON-RAPHSON ALGORITHM FOR
C    SOLVING SYSTEMS OF NONLINEAR ALGEBRAIC EQUATIONS.  A VARIATION OF
C    THE GAUSS-JORDAN MAXIMUM PIVOT STRATEGY IS EMPLOYED TO DETERMINE
C    THE INVERSE OF THE JACOBIAN MATRIX.  THE CORRECTION FACTORS ARE
C    CALCULATED IN AN ITERATIVE MANNER TO BRING THE ADJUSTABLE VARIABLES
C    WITHIN A SPECIFIED TOLERANCE.
C
C                   M = NUMBER OF COLUMNS IN MATRIX C
```

```
C                 N = NUMBER OF ROWS IN MATRIX C
C
C
C*************************************************************************
      SUBROUTINE XLIQUID(NC,MDL,MODEL,IOUT,NDIF,NACT,RI,QI,AI,MAIN)
C*************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*25 NAME
      DIMENSION C(10,11),XNEW(10),DX(10),IR(10),F(10),XMW(10),
     &          X1(10),X2(10),XOLD(10),FOLD(10),TEST(10),IE(10),
     &          ACT1(10),DACT1(10,10),TACT1(10),DLACT1(10),
     &          ACT2(10),DACT2(10,10),TACT2(10),DLACT2(10),
     &          XE(10,2),TEMP(10),FMIN(10,2),NAME(10),
     &          AI(40,40),RI(76),QI(76),MAIN(76)
C
C        --- SET LENGTH AND WIDTH OF JACOBIAN MATRIX ---
C
      N=NC
      M=N+1
      INDEX=0
C
C        --- INITIALIZE ARRAYS, VECTORS ---
C
      DO 5 I=1,10
C
         DO 6 J=1,N
            XE(I,J)=0.DO
            FMIN(I,J)=0.DO
    6    CONTINUE
C
         TEMP(I)=0.DO
         NAME(I)=' '
    5 CONTINUE
C
C        --- BEGIN OUTER LOOP TO READ MULTIPLE DATA SETS ---
C
      READ(6,*) IMAX,TOL
C
      WRITE(*,'(1X,A\)') 'Enter number of data sets (binary pairs) ==> '
      READ(*,'(BN,I3)') NDS
      WRITE(*,'(/)')
C
      DO 777 KN=1,NDS
C
C        --- READ DEFAULT PARAMETERS ---
C
      WRITE(*,'(1X,A,I2,A\)') 'Give name (<25 chars.) of binary system',
     &KN,' ==> '
      READ(*,'(BN,A)') NAME(KN)
      WRITE(*,'(/)')
C
      WRITE(*,'(1X,A\)') 'Enter absolute temperature in [K] ==> '
      READ(*,*) TEMP(KN)
```

```
         T=TEMP(KN)
      WRITE(*,'(/)')
C
      WRITE(7,902) KN,NAME(KN),TEMP(KN)
      WRITE(*,902) KN,NAME(KN),TEMP(KN)
      WRITE(7,903)
      WRITE(*,903)
C
      DO 7 LP=1,N
      WRITE(*,'(5X,A,I2,A\)') 'Enter molecular weight for component',LP,
     &' ==> '
      READ(*,*) XMW(LP)
C
      WRITE(*,'(5X,A,I2,A\)') 'Enter composition guess for component',
     &LP,' ==> '
      READ(*,*) XNEW(LP)
      WRITE(*,'(/)')
    7 CONTINUE
      WRITE(*,'(/)')
C
         CALL FINOUT(NC,RI,QI,AI,MAIN,NG)
         REWIND 8
C
C        --- INITIALIZE COEFFICIENT MATRICES (C,FOLD,XOLD,DX,IE) ---
C
      DO 10 L=1,N
         FOLD(L)=0.D0
         XOLD(L)=XNEW(L)
         DX(L)=0.D0
         IE(L)=0
C
            DO 20 LL=1,M
               C(L,LL)=0.D0
   20       CONTINUE
C
   10 CONTINUE
C
C        --- WRITE "WAIT" MESSAGE TO SCREEN ---
C
      WRITE(7,904)
      WRITE(*,904)
C
C
C        <<< START OF NEWTON-RAPHSON ITERATION LOOP >>>
C
C
      DO 999 ITER=1,IMAX
         INDEX=ITER-1
C
         WRITE(7,905) INDEX
         WRITE(*,905) INDEX
C
C        --- EVALUATE FUNCTION VECTOR (F) --
```

```
C
      X1(1)=XNEW(1)
      X1(2)=1.DO-X1(1)
      X2(1)=XNEW(2)
      X2(2)=1.DO-X2(1)
C
      CALL PARAM(N,NG,T)
      CALL UNIFA(NDIF,NACT,N,NG,T,X1,ACT1,DACT1,TACT1)
      CALL UNIFA(NDIF,NACT,N,NG,T,X2,ACT2,DACT2,TACT2)
C
      DO 21 J=1,N
         F(J)=X1(J)*ACT1(J)-X2(J)*ACT2(J)
         TEST(J)=DSQRT((FOLD(J))**2+(F(J))**2)
   21 CONTINUE
C
C     --- TEST FOR CONVERGENCE OF SOLUTION ---
C
      LOGIC=-1
      DIFF=DSQRT((XNEW(1)-XOLD(1))**2+(XNEW(2)-XOLD(2))**2)
      IF(DIFF.GT.TOL) LOGIC=1
C
      DO 22 I=1,N
         IF(TEST(I).GT.TOL) LOGIC=1
         IF(DX(I).GT.TOL) LOGIC=1
   22 CONTINUE
C
      IF(LOGIC.LT.0) GOTO 8
C
      DO 25 I=1,N
         FOLD(I)=F(I)
         XOLD(I)=XNEW(I)
   25 CONTINUE
C
C     --- CALCULATE PARTIAL DERIVATIVES IN JACOBIAN ---
C
      C(1,1)= ACT1(1)+XNEW(1)*DACT1(1,1)
      C(1,2)=-ACT2(1)-XNEW(2)*DACT2(1,1)
      C(2,1)=-ACT1(2)+(1.DO-XNEW(1))*DACT1(2,1)
      C(2,2)= ACT2(2)-(1.DO-XNEW(2))*DACT2(2,1)
C
C     --- FINISH LOADING C MATRIX WITH F VECTOR ---
C
      DO 30 I=1,N
         C(I,M)=-F(I)
   30 CONTINUE
C
C     *** GAUSS-JORDAN ALGORITHM ***
C
C
C     --- INITIALIZE ALL VECTORS AND MATRICES ---
C
      DO 40 I=1,N
         IR(I)=0
```

```
            DX(I)=0.D0
            JJ=0
            JM=0
   40   CONTINUE
C
        DO 50 K=1,N
            PK=0.D0
C
C       --- LOCATE PIVOT ELEMENT ---
C
            DO 60 I=1,N
                IF(I.EQ.IR(I)) GOTO 60
C
                DO 70 IK=1,N
                    P=DABS(C(I,IK))
                    IF(P.LT.PK) GOTO 70
                    PK=P
                    JJ=I
                    JM=IK
   70           CONTINUE
C
   60       CONTINUE
C
            IR(JJ)=JJ
C
C       --- NORMALIZATION STEP ---
C
            DO 80 JR=1,M
                IF(JM.EQ.JR) GOTO 80
                C(JJ,JR)=C(JJ,JR)/C(JJ,JM)
   80       CONTINUE
C
            C(JJ,JM)=1.D0
C
C       --- REDUCTION STEP ---
C
            DO 90 I=1,N
                IF(I.EQ.JJ) GOTO 90
C
                DO 100 JR=1,M
                    IF(JR.EQ.JM) GOTO 100
                    C(I,JR)=C(I,JR)-C(I,JM)*C(JJ,JR)
  100           CONTINUE
C
                C(I,JM)=0.D0
   90       CONTINUE
C
   50   CONTINUE
C
C       *** END GAUSS-JORDAN MAXIMUM PIVOT ROUTINE ***
C
C
C       --- RECOVER SOLUTION VECTOR --
```

```
C
        DO 110 I=1,N
C
           DO 120 J=1,N
              IF((C(I,J).LT.1.DO).OR.(C(I,J).GT.1.DO)) GOTO 120
              DX(J)=C(I,M)
  120      CONTINUE
C
  110   CONTINUE
C
C       --- CORRECT ELEMENTS OF X VECTOR ---
C
        DO 130 I=1,N
           XNEW(I)=XNEW(I)+DX(I)
           IF(XNEW(I).LT.0.DO) XNEW(I)=0.DO
           IF(XNEW(I).GT.1.DO) XNEW(I)=1.DO
  130   CONTINUE
C
  999 CONTINUE
C
      GOTO 9
C
C       <<< END OF ITERATION LOOP >>>
C
C
C       --- PRINT FINAL MATRIX (C) AND SOLUTION VECTOR ---
C
    8 WRITE(*,906) INDEX
      WRITE(7,906) INDEX
C
      DO 140 I=1,N
         WRITE(7,907) (C(I,J),J=1,N),C(I,M)
         WRITE(*,907) (C(I,J),J=1,N),C(I,M)
  140 CONTINUE
C
      WRITE(7,908)
      WRITE(*,908)
C
      DO 150 I=1,N
         WRITE(7,909) I,XNEW(I),I,F(I)
         WRITE(*,909) I,XNEW(I),I,F(I)
  150 CONTINUE
C
      WRITE(7,910)
      WRITE(*,910)
C
C       --- LOAD SUMMARY VECTORS FOR FINAL RESULTS TABLE ---
C
      DO 160 I=1,N
         DO 155 J=1,N
            IF(J.NE.I) GOTO 152
            IE(J)=IE(J)+1
  152       IF(XNEW(J).GT.XNEW(I)) IE(J)=IE(J)+1
```

```
  155     CONTINUE
C
          FMIN(KN,I)=F(I)
  160 CONTINUE
C
C         --- SORT COMPOSITION SUMMARY VECTOR ---
C
      DO 165 I=1,N
         XE(KN,I)=XNEW(IE(I))
  165 CONTINUE
C
C         --- CONVERT AQUEOUS CONCENTRATION TO PPMW UNITS ---
C
      XE(KN,1)=1000000.DO/(1.DO+((1.DO/XE(KN,1))-1.DO)*XMW(2)/XMW(1))
C
      GOTO 777
C
C         --- CONVERGENCE FAILURE MESSAGE ---
C
    9 WRITE(*,911) IMAX
      WRITE(7,911) IMAX
      WRITE(7,910)
      WRITE(*,910)
C
C         --- LOAD SUMMARY VECTORS WITH DEFAULT VALUES ---
C
      DO 170 I=1,N
         XE(KN,I)=-999.DO
         FMIN(KN,I)=-999.DO
         IF(XNEW(1).LT.(1.DO-TOL)) GOTO 170
         XE(KN,I)=XNEW(I)
         FMIN(KN,I)=F(I)
  170 CONTINUE
C
  777 CONTINUE
C
C         --- PRINT TABLE OF FINAL MISCIBILITY VALUES ---
C
      WRITE(7,912)
      WRITE(*,912)
      WRITE(7,913)
      WRITE(*,913)
C
      DO 180 I=1,NDS
         WRITE(7,914) NAME(I),TEMP(I),(XE(I,J),J=1,N)
         WRITE(*,914) NAME(I),TEMP(I),(XE(I,J),J=1,N)
  180 CONTINUE
C
C     --- FORMAT STATEMENTS ---
C
  901 FORMAT(A25)
  902 FORMAT(//,5X,'DATA SET',I3,' : ',A25,' AT',F7.2,' K')
  903 FORMAT(5X,8('-'),6X,37('-'),//)
```

```
  904 FORMAT(//,20X,'PLEASE WAIT... CALCULATIONS PROCEEDING...',/)
  905 FORMAT(30X,'ITERATION ',I3)
  906 FORMAT(/,15X,'FINAL SOLUTION MATRIX:   (AFTER',I3,' ITERATIONS)',
     &/)
  907 FORMAT(15X,7E15.5)
  908 FORMAT(/,5X,'SOLUTION VECTOR:',15X,'FUNCTION VECTOR:',/)
  909 FORMAT(5X,'XNEW(',I2,') =',E11.5,10X,'F(',I2,') =',E11.5)
  910 FORMAT(///)
  911 FORMAT(/,15X,'ALGORITHM DID NOT CONVERGE AFTER',I4,' ITERATIONS'/
  912 FORMAT(/,8X,'SYSTEM',7X,'TEMP (K)',5X,'X1 (PPMW,  I)',5X,
     &'X1 (M-F,  II)')
  913 FORMAT(8X,6('-'),7X,8('-'),5X,12('-'),5X,12('-'),/)
  914 FORMAT(1X,A15,5X,F8.2,4X,F8.1,5X,1E17.5)
      RETURN
      END
C
C
C   **************************************************************************
C   *
C   *
C   *       <<< SUBROUTINE TO CALCULATE THE ACTIVITY COEFFICIENTS >>>
C   *
C   *
C   **************************************************************************
      SUBROUTINE UNIFA(NDIF,NACT,NC,NG,T,X,ACT,DACT,TACT)
C   **************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/UNIF/RT(10,10),QT(10,10),TAU(10,10),S(10,10),F 10),Q(10),
     *            R(10),P(10,10)
      DIMENSION X(10),GAM(10),ACT(10),DACT(10,10),THETA(10) 'HI(10),
     *RI(10),QI(10),QIL(10),RIL(10),QID(10),ETAL(10),TACT(1   ,U(10,10),
     *V(10,10),DETA(10),DS(10,10),ETA(10),TETAR(10),H3(10,1
C
      THETS=0.D0
      PHS=0.D0
C
      DO 10 I=1,NC
         THETA(I)=X(I)*Q(I)
         PHI(I)=R(I)*X(I)
         THETS=THETS+THETA(I)
         PHS=PHS+PHI(I)
   10 CONTINUE
C
      DO 20 I=1,NC
         THETA(I)=THETA(I)/THETS
         PHI(I)=PHI(I)/PHS
         RI(I)=R(I)/PHS
         RIL(I)=DLOG(RI(I))
         QI(I)=Q(I)/THETS
         QID(I)=1.D0-RI(I)/QI(I)
         QIL(I)=DLOG(QI(I))
   20 CONTINUE
C
```

```fortran
      DO 30 I=1,NC
         XX=F(I)+Q(I)*(1.DO-QIL(I))-RI(I)+RIL(I)
         XX=XX-5.DO*Q(I)*(QID(I)+RIL(I)-QIL(I))
         GAM(I)=XX
   30 CONTINUE
C
      DO 50 I=1,NG
         TETAR(I)=0.DO
         ETA(I)=0.DO
C
         DO 40 J=1,NC
            ETA(I)=ETA(I)+S(I,J)*X(J)
            TETAR(I)=TETAR(I)+QT(I,J)*X(J)
   40    CONTINUE
C
         ETAL(I)=DLOG(ETA(I))
   50 CONTINUE
C
      DO 70 I=1,NC
C
         DO 60 J=1,NG
            U(J,I)=S(J,I)/ETA(J)
            V(J,I)=U(J,I)*TETAR(J)
            GAM(I)=GAM(I)-V(J,I)-QT(J,I)*ETAL(J)
   60    CONTINUE
C
         ACT(I)=DEXP(GAM(I))
         IF(NACT.EQ.1) ACT(I)=ACT(I)*X(I)
   70 CONTINUE
C
      IF(NDIF.EQ.0) GO TO 160
      IF(NDIF.EQ.2) GO TO 110
C
      DO 90 I=1,NC
      DO 90 J=1,NC
         XX=Q(I)*QI(J)*(1.DO-5.DO*QID(I)*QID(J))+(1.DO-RI(I))*
     &      (1.DO-RI(J))
C
         DO 80 K=1,NG
            XX=XX+U(K,I)*(V(K,J)-QT(K,J))-U(K,J)*QT(K,I)
   80    CONTINUE
C
         DACT(I,J)=XX
         DACT(J,I)=XX
         IF(NACT.EQ.1) GO TO 90
         DACT(I,J)=DACT(I,J)*ACT(I)
         IF(J.EQ.I) GO TO 90
         DACT(J,I)=DACT(J,I)*ACT(J)
   90 CONTINUE
C
      IF(NACT.EQ.0) GO TO 110
C
      DO 100 I=1,NC
```

```
      DO 100 J=1,NC
         DACT(I,J)=ACT(I)*(DACT(I,J)-1.DO)
         IF(J.EQ.I) DACT(I,J)=DACT(I,J)+DEXP(GAM(I))
  100 CONTINUE
  110 CONTINUE
C
      IF(NDIF.EQ.1) GO TO 160
C
      DO 130 K=1,NG
         DETA(K)=0.DO
      DO 130 I=1,NC
         DS(K,I)=0.DO
C
         DO 120 M=1,NG
            IF(QT(M,I).EQ.0.DO) GO TO 120
            DS(K,I)=DS(K,I)-QT(M,I)*DLOG(TAU(M,K))*TAU(M,K)/T
  120    CONTINUE
C
         DETA(K)=DETA(K)+DS(K,I)*X(I)
  130 CONTINUE
C
      DO 150 I=1,NC
         TACT(I)=0.DO
C
         DO 140 K=1,NG
            H3(K,I)=(-S(K,I)*DETA(K)/ETA(K)+DS(K,I))/ETA(K)
            HH=H3(K,I)*(TETAR(K)-QT(K,I)*ETA(K)/S(K,I))
            TACT(I)=TACT(I)-HH
  140    CONTINUE
C
         TACT(I)=TACT(I)*ACT(I)
  150 CONTINUE
  160 CONTINUE
      RETURN
      END
C
C
C  ********************************************************************
C  *                                                                  *
C  *                                                                  *
C  *       PARAM CALCULATES SOME COMPOSITION-INDEPENDENT QUANTITIES:  *
C  *       TAU, S, AND F, TO BE USED IN UNIFA.  PARAM MUST BE CALLED  *
C  *       PRIOR TO UNIFA.                                            *
C  *                                                                  *
C  *                                                                  *
C  ********************************************************************
      SUBROUTINE PARAM(NC,NG,T)
C  ********************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/UNIF/RT(10,10),QT(10,10),TAU(10,10),S(10,10),F(10),Q(10),
     *            R(10),P(10,10)
C
      DO 10 I=1,NG
```

```
      DO 10 J=1,NG
         TAU(I,J)=DEXP(-P(I,J)/T)
   10 CONTINUE
C
      DO 20 I=1,NC
      DO 20 K=1,NG
         S(K,I)=0.DO
      DO 20 M=1,NG
         S(K,I)=S(K,I)+QT(M,I)*TAU(M,K)
   20 CONTINUE
C
      DO 30 I=1,NC
         F(I)=1.DO
      DO 30 J=1,NG
         F(I)=F(I)+QT(J,I)*DLOG(S(J,I))
   30 CONTINUE
C
      RETURN
      END
C
C
C     ***********************************************************************
C     *                                                                     *
C     *                                                                     *
C     *         UVLE CONTAINS BUILT-IN UNIFAC VLE-PARAMETERS                *
C     *                                                                     *
C     *                                                                     *
C     ***********************************************************************
      SUBROUTINE UVLE(RI,QI,AI,MAIN)
C     ***********************************************************************
C
C     THE MAIN GROUPS ARE:
C      1 CH2 ....... 2 C=C ...... 3 ACH ...... 4 ACCH2 .... 5 OH .......
C      6 CH3OH ..... 7 H2O ...... 8 ACOH ..... 9 CH2CO ... 10 CHO ......
C     11 CCOO ..... 12 HCOO .... 13 CH2O .... 14 CNH2 .... 15 CNH ......
C     16 (C)3N .... 17 ACNH2 ... 18 PYRIDINE  19 CCN ..... 20 COOH .....
C     21 CCL ...... 22 CCL2 .... 23 CCL3 .... 24 CCL4 .... 25 ACCL .....
C     26 CNO2 ..... 27 ACNO2 ... 28 CS2 ..... 29 CH3SH ... 30 FURFURAL .
C     31 DOH ...... 32 I ....... 33 BR ...... 34 C=-C .... 35 DMSO .....
C     36 ACRY ..... 37 CLCC .... 38 ACF ..... 39 DMF ..... 40 CF2 ......
C
C
C     THE SUB GROUPS ARE:
C      1 CH3 ....... 2 CH2 ...... 3 CH ....... 4 C ........ 5 CH2=CH ...
C      6 CH=CH ..... 7 CH2=C .... 8 CH=C ..... 9 C=C ..... 10 ACH ......
C     11 AC ....... 12 ACCH3 ... 13 ACCH2 ... 14 ACCH .... 15 OH .......
C     16 CH3OH .... 17 H2O ..... 18 ACOH .... 19 CH3CO ... 20 CH2CO ....
C     21 CHO ...... 22 CH3COO .. 23 CH2COO .. 24 HCOO .... 25 CH3O .....
C     26 CH2O ..... 27 CH-O .... 28 FCH2O ... 29 CH3NH2 .. 30 CH2NH2 ...
C     31 CHNH2 .... 32 CH3NH ... 33 CH2NH ... 34 CHNH .... 35 CH3N .....
C     36 CH2N ..... 37 ACNH2 ... 38 C5H5N ... 39 C5H4N ... 40 C5H3N ....
C     41 CH3CN .... 42 CH2CN ... 43 COOH .... 44 HCOOH ... 45 CH2CL ....
C     46 CHCL ..... 47 CCL ..... 48 CH2CL2 .. 49 CHCL2 ... 50 CCL2 .....
```

```
C     51 CHCL3 .... 52 CCL3 .... 53 CCL4 .... 54 ACCL .... 55 CH3NO2 ...
C     56 CH2NO2 ... 57 CHNO2 ... 58 ACNO2 ... 59 CS2 ..... 60 CH3SH ....
C     61 CH2SH .... 62 FURFURAL  63 (CH2OH)2  64 I ....... 65 BR .......
C     66 CH=-C .... 67 C=-C .... 68 DMSO .... 69 ACRY .... 70 CL(C=-C) .
C     71 ACF ...... 72 DMF-1 ... 73 DMF-2 ... 74 CF3 ..... 75 CF2 ......
C     76 CF .......
C
C**********************************************************************
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/UNIF/RT(10,10),QT(10,10),TAU(10,10),S(10,10),F(10),Q(10),
     *            R(10),P(10,10)
      DIMENSION AI(40,40),RR(76),QQ(76),RI(76),QI(76),MAINSG(76),
     *          MAIN(76)
C
      DATA MAINSG/ 4*1, 5*2, 2*3, 3*4, 1*5, 1*6, 1*7, 1*8, 2*9,1*10,
     *            2*11,1*12,4*13,3*14,3*15,2*16,1*17,3*18,2*19,2*20,
     *            3*21,3*22,2*23,1*24,1*25,3*26,1*27,1*28,2*29,1*30,
     *            1*31,1*32,1*33,2*34,1*35,1*36,1*37,1*38,2*39,3*40/
C
      DATA RR/0.9011,0.6744,0.4469,0.2195,1.3454,1.1167,1.1173,0.8886,
     *0.6605,0.5313,0.3652,1.2663,1.0396,0.8121,1.0,1.4311,0.92,0.8952,
     *1.6724,1.4457,0.9980,1.9031,1.6764,1.2420,1.1450,0.9183,0.6908,
     *0.9183,1.5959,1.3692,1.1417,1.4337,1.2070,0.9795,1.1865,0.9597,
     *1.0600,2.9993,2.8332,2.6670,1.8701,1.6434,1.3013,1.5280,1.4654,
     *1.2380,1.0060,2.2564,2.0606,1.8016,2.8700,2.6401,3.3900,1.1562,
     *2.0086,1.7818,1.5544,1.4199,2.0570,1.8770,1.6510,3.1680,2.4088,
     *1.2640,0.9492,1.2920,1.0613,2.8266,2.3144,0.7910,0.6948,3.0856,
     *2.6322,1.4060,1.0105,0.6150/
C
      DATA QQ/0.848,0.540,0.228,0.000,1.176,0.867,0.988,0.676,0.485,
     *0.400,0.120,0.968,0.660,0.348,1.200,1.432,1.400,0.680,1.488,
     *1.180,0.948,1.728,1.420,1.188,1.088,0.780,0.468,1.100,1.544,
     *1.236,0.924,1.244,0.936,0.624,0.940,0.632,0.816,2.113,1.833,
     *1.553,1.724,1.416,1.224,1.532,1.264,0.952,0.724,1.988,1.684,
     *1.448,2.410,2.184,2.910,0.844,1.868,1.560,1.248,1.104,1.650,
     *1.676,1.368,2.481,2.248,0.992,0.832,1.088,0.784,2.472,2.052,
     *0.724,0.524,2.736,2.120,1.380,0.920,0.460/
C
      OPEN(9,FILE='AVLE.DAT',STATUS='OLD',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
      OPEN(10,FILE='AVLE.OUT',STATUS='NEW',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
C
      DO 5 I=1,76
         RI(I)=0.D0
         QI(I)=0.D0
         MAIN(I)=0.D0
    5 CONTINUE
C
      DO 20 I=1,40
         DO 10 J=1,40
            AI(I,J)=0.D0
```

```
   10     CONTINUE
   20 CONTINUE
C
      DO 40 I=1,40
         DO 30 J=1,8
            READ(9,*,END=40) (AI((5*(J-1)+K),I), K=1,5)
   30    CONTINUE
   40 CONTINUE
C
      DO 50 I=1,76
         RI(I)=RR(I)
         QI(I)=QQ(I)
         MAIN(I)=MAINSG(I)
   50 CONTINUE
C
      DO 70 I=1,40
         DO 60 J=1,8
            WRITE(10,999) (AI((5*(J-1)+K),I), K=1,5)
   60    CONTINUE
   70 CONTINUE
C
C        --- FORMAT STATEMENTS ---
C
  999 FORMAT(5F10.3)
C
      RETURN
      END
C
C
C  *******************************************************************
C  *                                                                 *
C  *                                                                 *
C  *           ULLE CONTAINS BUILT-IN UNIFAC LLE-PARAMETERS          *
C  *                                                                 *
C  *                                                                 *
C  *******************************************************************
      SUBROUTINE ULLE(RI,QI,AI,MAIN)
C  *******************************************************************
C
C     THE MAIN GROUPS ARE:
C      1 CH2 ....... 2 C=C ...... 3 ACH ...... 4 ACCH2 .... 5 OH .......
C      6 P1 ........ 7 P2 ....... 8 H2O ...... 9 ACOH .... 10 CH2CO ....
C     11 CHO ...... 12 FURFURAL  13 COOH .... 14 COOC .... 15 CH2O .....
C     16 CCL ...... 17 CCL2 .... 18 CCL3 .... 19 CCL4 .... 20 ACCL .....
C     21 CCN ...... 22 ACNH2 ... 23 CNO2 .... 24 ACNO2 ... 25 DOH ......
C     26 DEOH ..... 27 PYRIDINE  28 TCE ..... 29 MFA ..... 30 DMFA .....
C     31 TMS ...... 32 DMSO ....
C
C
C     THE SUB GROUPS ARE:
C      1 CH3 ....... 2 CH2 ...... 3 CH ....... 4 C ........ 5 CH2=CH ...
C      6 CH=CH ..... 7 CH=C ..... 8 CH2=C .... 9 ACH ..... 10 AC .......
C     11 ACCH3 .... 12 ACCH2 ... 13 ACCH .... 14 OH ...... 15 P1 .......
```

```
C      16 P2 ....... 17 H2O ..... 18 ACOH .... 19 CH3CO ... 20 CH2CO ...
C      21 CHO ...... 22 FURFURAL  23 COOH .... 24 HCOOH ... 25 CH3COO ..
C      26 CH2COO ... 27 CH3O .... 28 CH2O .... 29 CH-O .... 30 FCH2O ...
C      31 CH2CL .... 32 CHCL .... 33 CCL ..... 34 CH2CL2 .. 35 CHCL2 ...
C      36 CCL2 ..... 37 CHCL3 ... 38 CCL3 .... 39 CCL4 .... 40 ACCL ....
C      41 CH3CN .... 42 CH2CN ... 43 ACNH2 ... 44 CH3NO2 .. 45 CH2NO2 ..
C      46 CHNO2 .... 47 ACNO2 ... 48 (CH2OH)2  49 (HOMM)2O  50 C5H5N ...
C      51 C5H4N .... 52 C5H3N ... 53 CCL2=CHCL 54 HCONHCH3  55 HCON(CH3)
C      56 (CH2)4SO2  57 (CH2)2SO
C
C************************************************************************
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/UNIF/RT(10,10),QT(10,10),TAU(10,10),S(10,10),F(10),Q(10),
     *            R(10),P(10,10)
      DIMENSION AI(40,40),RR(57),QQ(57),RI(76),QI(76),MAINSG(57),
     *          MAIN(76)
C
      DATA MAINSG/ 4*1, 4*2, 2*3, 3*4, 1*5, 1*6, 1*7, 1*8, 1*9,2*10,
     *            1*11,1*12,2*13,2*14,4*15,3*16,3*17,2*18,1*19,1*20,
     *            2*21,1*22,3*23,1*24,1*25,1*26,3*27,1*28,1*29,1*30,
     *            1*31,1*32/
C
      DATA RR/0.9011,0.6744,0.4469,0.2195,1.3454,1.1167,0.8886,1.1173,
     *0.5313,0.3652,1.2663,1.0396,0.8121,1.0000,3.2499,3.2491,0.9200,
     *0.8952,1.6724,1.4457,0.9980,3.1680,1.3013,1.5280,1.9031,1.6764,
     *1.1450,0.9183,0.6908,0.9183,1.4654,1.2380,1.0060,2.2564,2.0606,
     *1.8016,2.8700,2.6401,3.3900,1.1562,1.8701,1.6434,1.0600,2.0086,
     *1.7818,1.5544,1.4199,2.4088,4.0013,2.9993,2.8332,2.6670,3.3092,
     *2.4317,3.0856,4.0358,2.8266/
C
      DATA QQ/0.848,0.540,0.228,0.000,1.176,0.867,0.676,0.988,0.400,
     *0.120,0.968,0.660,0.348,1.200,3.128,3.124,1.400,0.680,1.488,
     *1.180,0.948,2.484,1.224,1.532,1.728,1.420,1.088,0.780,0.468,
     *1.100,1.264,0.952,0.724,1.988,1.684,1.448,2.410,2.184,2.910,
     *0.844,1.724,1.416,0.816,1.868,1.560,1.248,1.104,2.248,3.568,
     *2.113,1.833,1.553,2.860,2.192,2.736,3.200,2.472/
C
      OPEN(11,FILE='ALLE.DAT',STATUS='OLD',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
      OPEN(12,FILE='ALLE.OUT',STATUS='NEW',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
C
      DO 5 I=1,76
         RI(I)=0.D0
         QI(I)=0.D0
         MAIN(I)=0.D0
    5 CONTINUE
C
      DO 20 I=1,40
         DO 10 J=1,40
            AI(I,J)=0.D0
   10    CONTINUE
```

```
   20 CONTINUE
C
      DO 40 I=1,32
         DO 30 J=1,6
            READ(11,*,END=40) (AI((5*(J-1)+K),I), K=1,5)
   30    CONTINUE
            READ(11,*,END=40) (AI(K,I), K=31,32)
   40 CONTINUE
C
      DO 50 I=1,57
         RI(I)=RR(I)
         QI(I)=QQ(I)
         MAIN(I)=MAINSG(I)
   50 CONTINUE
C
      DO 70 I=1,32
         DO 60 J=1,6
            WRITE(12,999) (AI((5*(J-1)+K),I), K=1,5)
   60    CONTINUE
            WRITE(12,999) (AI(K,I), K=31,32)
   70 CONTINUE
C
C        --- FORMAT STATEMENTS ---
C
  999 FORMAT(5F10.3)
C
      RETURN
      END
C
C
C  *******************************************************************
C  *                                                                 *
C  *                                                                 *
C  *      ENVIRON CONTAINS "ENVIRONMENTAL" UNIFAC VLE-PARAMETERS     *
C  *                                                                 *
C  *                                                                 *
C  *******************************************************************
      SUBROUTINE ENVIRON(RI,QI,AI,MAIN)
C  *******************************************************************
C
C     THE MAIN GROUPS ARE:
C      1 CH2 ....... 2 C=C ...... 3 ACH ...... 4 ACCH2 .... 5 OH .......
C      6 CH3OH ..... 7 H2O ...... 8 ACOH ..... 9 CH2CO ... 10 CHO ......
C     11 CCOO ..... 12 HCOO .... 13 CH2O .... 14 CNH2 .... 15 CNH ......
C     16 (C)3N .... 17 ACNH2 ... 18 PYRIDINE  19 CCN ..... 20 COOH .....
C     21 CCL ...... 22 CCL2 .... 23 CCL3 .... 24 CCL4 .... 25 ACCL .....
C     26 CNO2 ..... 27 ACNO2 ... 28 CS2 ..... 29 CH3SH ... 30 FURFURAL .
C     31 DOH ...... 32 I ....... 33 BR ...... 34 C=-C .... 35 DMSO .....
C     36 ACRY ..... 37 CLCC .... 38 ACF ..... 39 DMF ..... 40 CF2 ......
C
C
C     THE SUB GROUPS ARE:
C      1 CH3 ....... 2 CH2 ...... 3 CH ....... 4 C ........ 5 CH2=CH ...
```

```
C      6 CH=CH ..... 7 CH2=C .... 8 CH=C ..... 9 C=C ..... 10 ACH ......
C     11 AC ....... 12 ACCH3 ... 13 ACCH2 ... 14 ACCH .... 15 OH .......
C     16 CH3OH .... 17 H2O ..... 18 ACOH .... 19 CH3CO ... 20 CH2CO ....
C     21 CHO ...... 22 CH3COO .. 23 CH2COO .. 24 HCOO .... 25 CH3O .....
C     26 CH2O ..... 27 CH-O .... 28 FCH2O ... 29 CH3NH2 .. 30 CH2NH2 ...
C     31 CHNH2 .... 32 CH3NH ... 33 CH2NH ... 34 CHNH .... 35 CH3N .....
C     36 CH2N ..... 37 ACNH2 ... 38 C5H5N ... 39 C5H4N ... 40 C5H3N ....
C     41 CH3CN .... 42 CH2CN ... 43 COOH .... 44 HCOOH ... 45 CH2CL ....
C     46 CHCL ..... 47 CCL ..... 48 CH2CL2 .. 49 CHCL2 ... 50 CCL2 .....
C     51 CHCL3 .... 52 CCL3 .... 53 CCL4 .... 54 ACCL .... 55 CH3NO2 ...
C     56 CH2NO2 ... 57 CHNO2 ... 58 ACNO2 ... 59 CS2 ..... 60 CH3SH ....
C     61 CH2SH .... 62 FURFURAL  63 (CH2OH)2  64 I ....... 65 BR .......
C     66 CH=-C .... 67 C=-C .... 68 DMSO .... 69 ACRY .... 70 CL(C=-C) .
C     71 ACF ...... 72 DMF-1 ... 73 DMF-2 ... 74 CF3 ..... 75 CF2 ......
C     76 CF .......
C
C*********************************************************************
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/UNIF/RT(10,10),QT(10,10),TAU(10,10),S(10,10),F(10),Q(10),
     *            R(10),P(10,10)
      DIMENSION AI(40,40),RR(76),QQ(76),RI(76),QI(76),MAINSG(76),
     *          MAIN(76)
C
      DATA MAINSG/ 4*1, 5*2, 2*3, 3*4, 1*5, 1*6, 1*7, 1*8, 2*9,1*10,
     *            2*11,1*12,4*13,3*14,3*15,2*16,1*17,3*18,2*19,2*20,
     *            3*21,3*22,2*23,1*24,1*25,3*26,1*27,1*28,2*29,1*30,
     *            1*31,1*32,1*33,2*34,1*35,1*36,1*37,1*38,2*39,3*40/
C
      DATA RR/0.9011,0.6744,0.4469,0.2195,1.3454,1.1167,1.1173,0.8886,
     *0.6605,0.5313,0.3652,1.2663,1.0396,0.8121,1.0,1.4311,0.92,0.8952,
     *1.6724,1.4457,0.9980,1.9031,1.6764,1.2420,1.1450,0.9183,0.6908,
     *0.9183,1.5959,1.3692,1.1417,1.4337,1.2070,0.9795,1.1865,0.9597,
     *1.0600,2.9993,2.8332,2.6670,1.8701,1.6434,1.3013,1.5280,1.4654,
     *1.2380,1.0060,2.2564,2.0606,1.8016,2.8700,2.6401,3.3900,1.1562,
     *2.0086,1.7818,1.5544,1.4199,2.0570,1.8770,1.6510,3.1680,2.4088,
     *1.2640,0.9492,1.2920,1.0613,2.8266,2.3144,0.7910,0.6948,3.0856,
     *2.6322,1.4060,1.0105,0.6150/
C
      DATA QQ/0.848,0.540,0.228,0.000,1.176,0.867,0.988,0.676,0.485,
     *0.400,0.120,0.968,0.660,0.348,1.200,1.432,1.400,0.680,1.488,
     *1.180,0.948,1.728,1.420,1.188,1.088,0.780,0.468,1.100,1.544,
     *1.236,0.924,1.244,0.936,0.624,0.940,0.632,0.816,2.113,1.833,
     *1.553,1.724,1.416,1.224,1.532,1.264,0.952,0.724,1.988,1.684,
     *1.448,2.410,2.184,2.910,0.844,1.868,1.560,1.248,1.104,1.650,
     *1.676,1.368,2.481,2.248,0.992,0.832,1.088,0.784,2.472,2.052,
     *0.724,0.524,2.736,2.120,1.380,0.920,0.460/
C
      OPEN(13,FILE='AENV.DAT',STATUS='OLD',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
      OPEN(14,FILE='AENV.OUT',STATUS='NEW',ACCESS='SEQUENTIAL',
     +FORM='FORMATTED')
C
```

```
      DO 5 I=1,76
         RI(I)=0.D0
         QI(I)=0.D0
         MAIN(I)=0.D0
    5 CONTINUE
C
      DO 20 I=1,40
         DO 10 J=1,40
            AI(I,J)=0.D0
   10    CONTINUE
   20 CONTINUE
C
      DO 40 I=1,40
         DO 30 J=1,8
            READ(13,*,END=40) (AI((5*(J-1)+K),I), K=1,5)
   30    CONTINUE
   40 CONTINUE
C
      DO 50 I=1,76
         RI(I)=RR(I)
         QI(I)=QQ(I)
         MAIN(I)=MAINSG(I)
   50 CONTINUE
C
      DO 70 I=1,40
         DO 60 J=1,8
            WRITE(14,999) (AI((5*(J-1)+K),I), K=1,5)
   60    CONTINUE
   70 CONTINUE
C
C        --- FORMAT STATEMENTS ---
C
  999 FORMAT(5F10.3)
C
      RETURN
      END
```


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